specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:34:41 ON 14 SEP 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:34:51 ON 14 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 SEP 2007 HIGHEST RN 947061-18-9
DICTIONARY FILE UPDATES: 13 SEP 2007 HIGHEST RN 947061-18-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

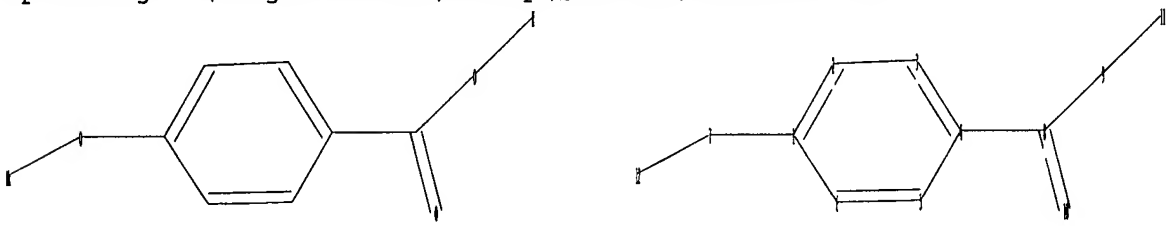
=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 2076

L1 SCREEN CREATED

=>
Uploading C:\Program Files\Stnexp\Queries\10594501c.str



chain nodes :
7 8 9 10 11 12
ring nodes :

1 2 3 4 5 6
chain bonds :
1-7 4-8 7-12 8-9 8-10 9-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-7 7-12
exact bonds :
4-8 9-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-10

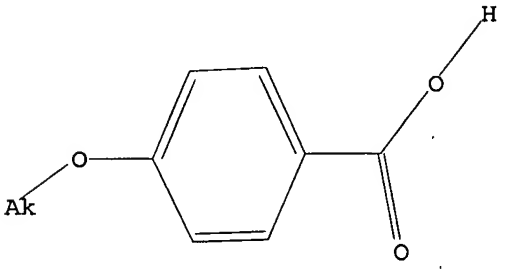
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom

L2 STRUCTURE UPLOADED

=> que L2 AND L1

L3 QUE L2 AND L1

=> d L2
L2 HAS NO ANSWERS
L2 STR



Structure attributes must be viewed using STN Express query preparation.

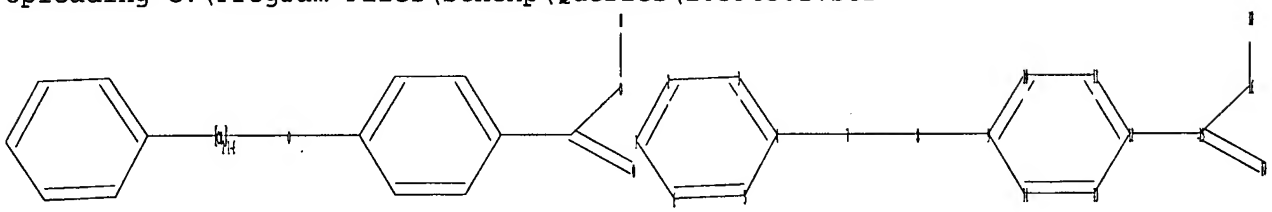
=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 2076

L4 SCREEN CREATED

=>
Uploading C:\Program Files\Stnexp\Queries\10594501.str



chain nodes :
7 8 15 16 17 18
ring nodes :
1 2 3 4 5 6 9 10 11 12 13 14
chain bonds :
4-7 7-8 8-9 12-15 15-16 15-17 16-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14
exact/norm bonds :
8-9
exact bonds :
4-7 7-8 12-15 16-18
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-17

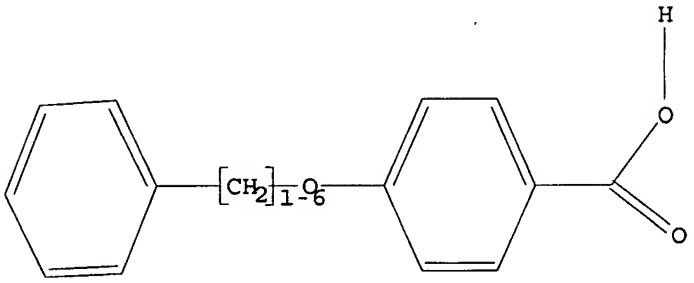
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom
18:Atom

L5 STRUCTURE UPLOADED

=> que L5 AND L4

L6 QUE L5 AND L4

=> d L5
L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L5 (w) L2
'W' IS NOT VALID FOR THIS COM

=> s L5 full
FULL SEARCH INITIATED 17:36:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 28787 TO ITERATE

100.0% PROCESSED 28787 ITERATIONS 1309 ANSWERS
SEARCH TIME: 00.00.01

L7 1309 SEA SSS FUL L5

=> s L2 full
FULL SEARCH INITIATED 17:36:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 190577 TO ITERATE

100.0% PROCESSED 190577 ITERATIONS 20757 ANSWERS
SEARCH TIME: 00.00.03

L8 20757 SEA SSS FUL L2

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 344.65 344.86

FILE 'CAPLUS' ENTERED AT 17:36:22 ON 14 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 14 Sep 2007 VOL 147 ISS 13
FILE LAST UPDATED: 13 Sep 2007 (20070913/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s L7
L9 1304 L7

=> s L8
L10 22966 L8

=> s L9 (w) L10
L11 0 L9 (W) L10

=> s process
  2488712 PROCESS
  1695330 PROCESSES
L12 3711754 PROCESS
  (PROCESS OR PROCESSES)

=> s L9 and L12
L13 72 L9 AND L12

=> s L10 and L12
L14 1376 L10 AND L12

=> s L13 and L14
L15 72 L13 AND L14

=> s phase separation
  1802002 PHASE
  371790 PHASES
  1958051 PHASE
  (PHASE OR PHASES)
  211663 SEPARATION

```
          7724 SEPARATIONS
        218012 SEPARATION
                 (SEPARATION OR SEPARATIONS)
        601109 SEPN
         38907 SEPNS
        620779 SEPN
                 (SEPN OR SEPNS)
        684173 SEPARATION
                 (SEPARATION OR SEPN)
L16      42056 PHASE SEPARATION
                 (PHASE(W)SEPARATION)

=> s L15 and L16
L17          0 L15 AND L16

=> d L15 1-72 bib abs hitstr

L15  ANSWER 1 OF 72  CAPLUS  COPYRIGHT 2007 ACS on STN
AN   2007:935084  CAPLUS
TI   Azacyclyl-substituted aryldihydroisoquinolinones as MCH antagonists,
     process for their preparation and their use as medicaments
IN   Schwink, Lothar; Stengelin, Siegfried; Gossel, Matthias; Hessler, Gerhard;
     Haack, Torsten; Lennig, Petra
PA   Sanofi-Aventis, Fr.
SO   PCT Int. Appl., 259pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
PI   WO 2007093364         A1    20070823    WO 2007-EP1212          20070213
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN,
             KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,
             MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO,
             RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRAI DE 2006-102006007045 A     20060215
GI
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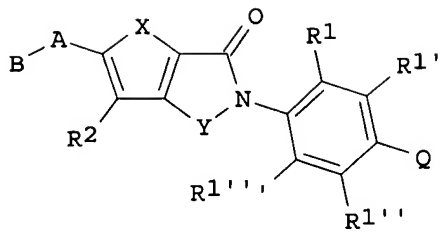
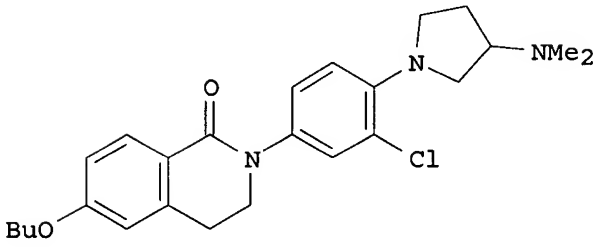


I



II

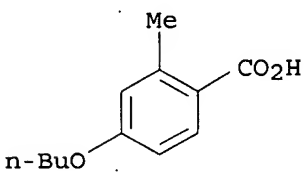
AB The invention relates to azacyclyl-substituted aryldihydroisoquinolinones of formula I and their derivs., and their physiol. tolerated salts and physiol. functional derivs., their preparation, medicaments comprising at least one azacyclyl-substituted aryldihydroisoquinolinone of the invention or its derivative, and the use of the azacyclyl-substituted aryldihydroisoquinolinones of the invention and their derivs. as MCH antagonists. Compds. of formula I wherein R1, R1', R1'', R1''' and R2 are independently H, F, Cl, Br, I, OH and derivs., CF3, NO2, CN, OCF3, etc.; X is S, O, and (un)substituted ethylene; A is a bond an a 1- to 8-membered linker; B is H,NH2 and derivs.m HO-C1-4 alkyl, C1-8 alkyl, C2-8 alkenyl, etc.; Y is (un)substituted Et and (un)substituted ethylene; Q is (un)substituted (un)saturated (mono/bi/tri/spiro)azacyclyl; and their method for preparation are claimed. Example compound II was prepared by a multistep procedure (procedure given). All the invention compds. were evaluated for their MCH antagonistic activity. From the assay, it was determined that compound II exhibited an IC50 value of 0.99 μM.

IT INDEXING IN PROGRESS

IT 175153-56-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of azacyclyl-substituted aryldihydroisoquinolinones as MCH antagonists)

RN 175153-56-7 CAPLUS

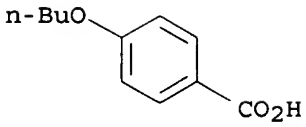
CN Benzoic acid, 4-butoxy-2-methyl- (CA INDEX NAME)



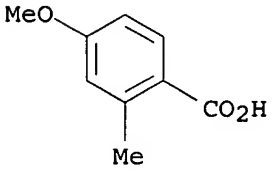
IT 1498-96-0, 4-Butoxybenzoic acid 6245-57-4, 4-Methoxy-2-methylbenzoic acid 17819-91-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of azacyclyl-substituted aryldihydroisoquinolinones as MCH antagonists)

RN 1498-96-0 CAPLUS

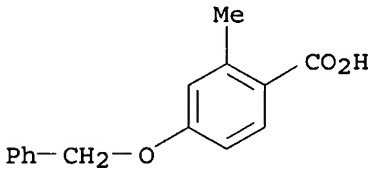
CN Benzoic acid, 4-butoxy- (CA INDEX NAME)



RN 6245-57-4 CAPLUS
CN Benzoic acid, 4-methoxy-2-methyl- (CA INDEX NAME)



RN 17819-91-9 CAPLUS
CN Benzoic acid, 2-methyl-4-(phenylmethoxy)- (CA INDEX NAME)

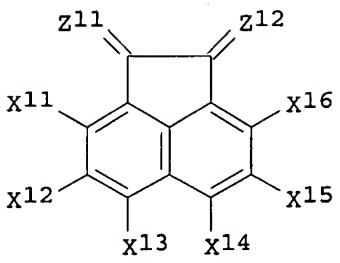


RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:759265 CAPLUS
DN 147:176996
TI Electrophotographic photoconductor, process cartridges, and electrophotographic apparatus
IN Sekiya, Michiyo; Nagasaka, Hideaki; Sekido, Kunihiko; Fukaya, Kunihisa
PA Canon Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 31pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2007179031	A	20070712	JP 2006-321761	20061129
PRAI	JP 2005-346210	A	20051130		

GI



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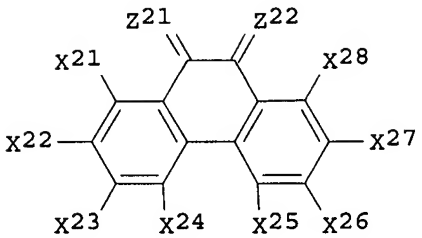
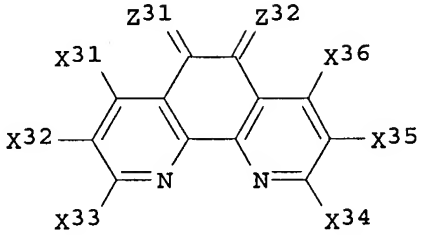


II



III

AB The electrophotog. photoconductors contain polymers of I, II, and III [Z11, Z12, Z21, Z22, Z31, Z32 = O, C(CN)2, NR, C(CN)COR, C(CN)CO2R, C(CN)R, C(CO2R)2; R = (un)substituted aryl or alkyl; where ≥1 of X11-X16, X21-X28, and X31-X36 being a polymerizable group, and the other groups being H, halo, NO2, trifluoroalkyl, (un)substituted alkoxy or alkyl] as electron transport materials. The photoconductors show potential stability under low-temperature and low-humidity conditions, and are capable of producing high-quality images.

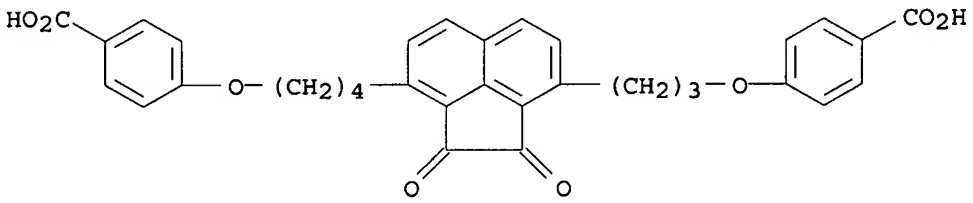
IT 943862-14-4
RL: TEM (Technical or engineered material use); USES (Uses)
(electron transport materials for electrophotog. photoconductors)

RN 943862-14-4 CAPLUS

CN Benzoic acid, 4-[3-[8-[4-(4-carboxyphenoxy)butyl]-1,2-dihydro-1,2-dioxo-3-acenaphthylenyl]propoxy]-, polymer with formaldehyde and 1,3,5-triazine-2,4,6-triamine (CA INDEX NAME)

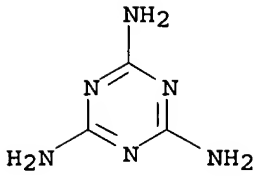
CM 1

CRN 943862-13-3
CMF C33 H28 O8



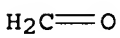
CM 2

CRN 108-78-1
CMF C3 H6 N6

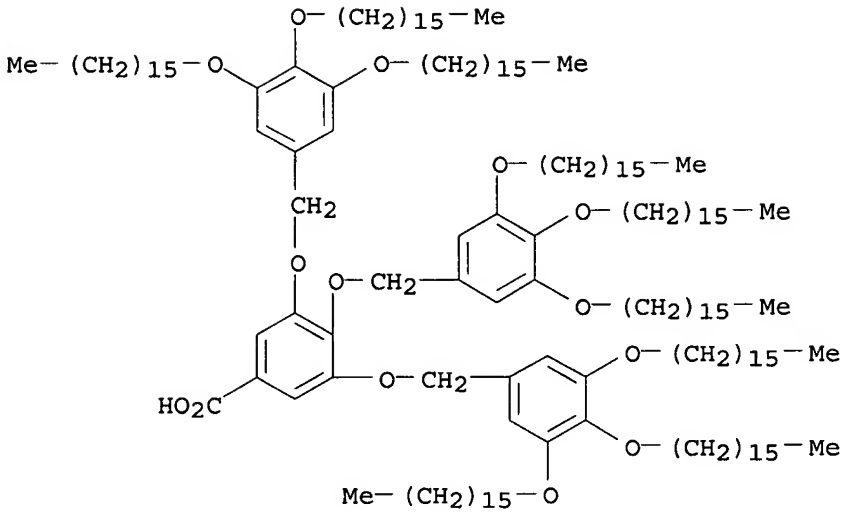


CM 3

CRN 50-00-0
CMF C H2 O



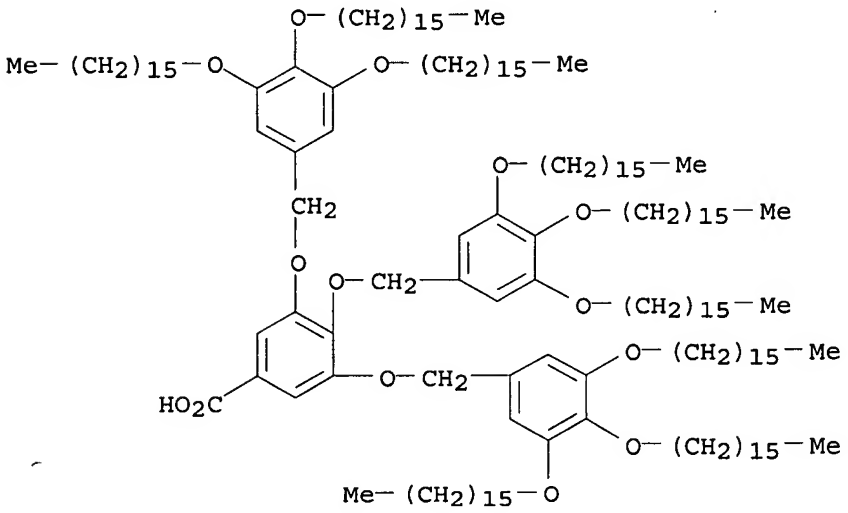
L15 ANSWER 3 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:626018 CAPLUS
DN 147:235619
TI Hierarchical self-assembling of dendritic-linear diblock complex based on hydrogen bonding
AU Liu, Qingtao; Zhang, Hui; Yin, Shengyan; Wu, Lixin; Shao, Chen; Su, Zhongmin
CS Key Laboratory for Supramolecular Structure and Materials of Ministry of Education, Jilin University, Changchun, 130012, Peop. Rep. China
SO Polymer (2007), 48(13), 3759-3770
CODEN: POLMAG; ISSN: 0032-3861
PB Elsevier Ltd.
DT Journal
LA English
AB An effective route was demonstrated to fabricate vesicles, cylindrical micelles, fibers and hierarchical structures by using dendritic-linear amphiphilic diblock complex as building block through hydrogen bonding. We tailored the formation and evolution of these aggregation morphologies as well as the transformation among them, and found that the concentration and solvent polarity could affect the aggregation states of the complex in solution and the self-assembling process on solid substrate. Addnl., the flexible-rigid structure of the complex and the template effect of DMSO droplets resulting from solvent evaporation also play important roles in constructing higher level organized structures such as hierarchical wreath-like and hollow entanglement self-assemblies at solid-gas interface. The cast film of the complex which possesses a fibrous structure shows superhydrophobicity and when the solution was allowed to stand for some days, a transparent organic gel spontaneously formed from the mixed solution Based on the experiment results, the hierarchical architectures are proposed to derive from primary fibrils. The structure of the cylindrical micelle is believed to possess an alkyl chain block shell and a poly(ethylene oxide) block core, which is consistent with the water contact angle measurement and the simulation to the volume ratio of the two blocks of the complex.
IT 945631-97-0 945631-98-1
RL: PRP (Properties)
(preparation and hierarchical self-assembling of dendritic-linear diblock complex based on hydrogen bonding)
RN 945631-97-0 CAPLUS
CN Benzoic acid, 3,4,5-tris[[3,4,5-tris(hexadecyloxy)phenyl]methoxy]- (CA INDEX NAME)



RN 945631-98-1 CAPLUS
CN Benzoic acid, 3,4,5-tris[[3,4,5-tris(hexadecyloxy)phenyl]methoxy]-, compd. with α-methyl-ω-[4-[(1E)-2-(4-pyridinyl)ethenyl]phenoxy]poly(oxy-1,2-ethanediyl) (1:1) (CA INDEX NAME)

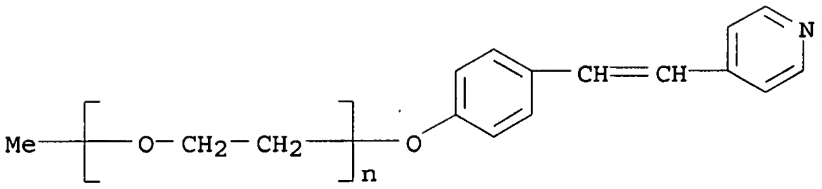
CM 1

CRN 945631-97-0
CMF C172 H312 O14



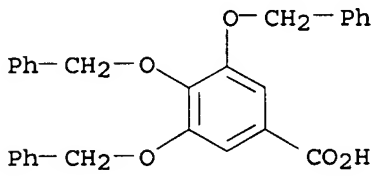
CM 2

CRN 945631-96-9
CMF (C2 H4 O)n C14 H13 N O
CCI PMS



RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:454119 CAPLUS
DN 147:97314
TI Scale-Up Syntheses of Two Naturally Occurring Procyanidins: (-)-Epicatechin-(4β,8)-(+)-catechin and (-)-Epicatechin-3-O-galloyl-(4β,8)-(-)-epicatechin-3-O-gallate
AU Sharma, Pradeep K.; Kolchinski, Alexander; Shea, Helene A.; Nair, Jayesh J.; Gou, Yanni; Romanczyk, Leo J., Jr.; Schmitz, Harold H.
CS Chemical Process Research & Development, Catalytic Services, and Analytical Division, Johnson Matthey Pharmaceutical Materials, Inc., Devens, MA, 01434, USA
SO Organic Process Research & Development (2007), 11(3), 422-430
CODEN: OPRDFK; ISSN: 1083-6160
PB American Chemical Society
DT Journal
LA English
AB A scaleable process for the synthesis of two naturally occurring procyanidins, namely (-)-epicatechin-(4β,8)-(+)-catechin (1) and (-)-epicatechin-3-O-galloyl-(4β,8)-(-)-epicatechin-3-O-gallate (2), is described. The key steps were highlighted by improvements for the benzylation of (+)-catechin, stereoselective reduction of the C-3 keto group of (2R)-5,7,3',4'-tetrakis(benzyloxy)flavan-3-one, and coupling between 4-hydroxyethoxy-5,7,3',4'-tetra-O-benzyl-(-)-epicatechin and 5,7,3',4'-tetra-O-benzyl-(+)-catechin or 5,7,3',4'-tetra-O-benzyl-(-)-epicatechin, resp. The debenzylation performed in a biphasic system resulted in an improved yield and purity of the target compds. The chemical was scaled-up to produce multigram quantities of 1 and 2 for various in vitro, ex vivo, and in vivo studies. The scale-up process provided a detailed description for the preparation of multi-hundred to kilogram scale quantities of intermediates used in the synthesis of these two titled procyanidins.
IT 1486-48-2, Tri-O-benzylgallic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(improved steps and scale-up syntheses of (-)-epicatechin-(4β,8)-(+)-catechin and (-)-epicatechin-3-O-galloyl-(4β,8)-(-)-epicatechin-3-O-gallate)
RN 1486-48-2 CAPLUS
CN Benzoic acid, 3,4,5-tris(phenylmethoxy)- (CA INDEX NAME)



RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

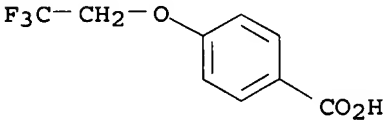
AN 2007:83819 CAPLUS
DN 146:184254
TI Preparation of benzamide derivatives for treatment of diseases related to bone metabolism
IN Aoki, Kazumasa; Suda, Koji; Gotanda, Kentoku; Kimura, Tomio
PA Sankyo Company, Limited, Japan
SO PCT Int. Appl., 246pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2007010885	A1	20070125	WO 2006-JP314144	20060718

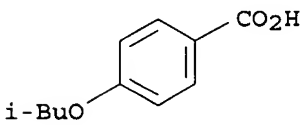
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI JP 2005-208036 A 20050719
OS MARPAT 146:184254
AB The title compds. R1CONHCH(COX)CH2R2 [R1 = (un)substituted aryl, (un)substituted 5- to 10-membered heteroaryl; R2 = (un)substituted aryl, (un)substituted 5- to 10-membered heteroaryl, etc.; X = OH, alkoxy group, etc.] are prepared 4-(2-Cyclopropylethoxy)-N-[2-[(2-hydroxyethyl)amino]-2-oxo-1-(4-propylbenzyl)ethyl]benzamide was prepared in a multistep process starting from 4-hydroxybenzoic acid Me ester and 2-cyclopropylethanol. In an assay using rats with adjuvant arthritis, compds. of this invention at 3 mg/kg gave 75% to 92% inhibition of bone d. decrease.
IT 27914-56-3 30762-00-6, 4-Isobutoxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzamide derivs. for treatment of diseases related to bone metabolism)
RN 27914-56-3 CAPLUS
CN Benzoic acid, 4-(2,2,2-trifluoroethoxy)- (CA INDEX NAME)



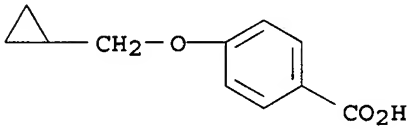
RN 30762-00-6 CAPLUS
CN Benzoic acid, 4-(2-methylpropoxy)- (CA INDEX NAME)



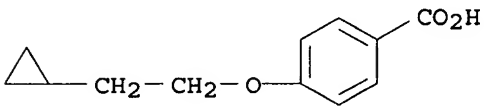
IT 355391-05-8P, 4-(Cyclopropylmethoxy)benzoic acid
915016-54-5P, 4-(2-Cyclopropylethoxy)benzoic acid
921622-91-5P, 4-[2-(4-Chlorophenyl)ethoxy]benzoic acid

921623-04-3P, 4-(2,2-Difluoroethoxy)benzoic acid
921623-07-6P 921623-15-6P, 4-[(2,2-
Difluorocyclopropyl)methoxy]benzoic acid 921623-31-6P,
4-(4,4,4-Trifluorobutoxy)benzoic acid 921623-34-9P,
2-Fluoro-4-(3,3,3-trifluoropropoxy)benzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzamide derivs. for treatment of diseases related to bone metabolism)

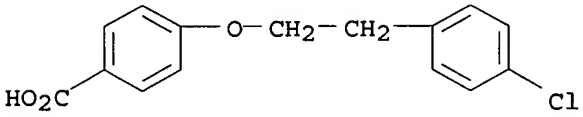
RN 355391-05-8 CAPLUS
CN Benzoic acid, 4-(cyclopropylmethoxy)- (CA INDEX NAME)



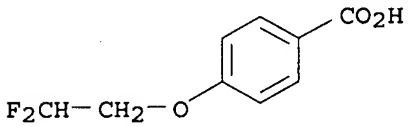
RN 915016-54-5 CAPLUS
CN Benzoic acid, 4-(2-cyclopropylethoxy)- (CA INDEX NAME)



RN 921622-91-5 CAPLUS
CN Benzoic acid, 4-[2-(4-chlorophenyl)ethoxy]- (CA INDEX NAME)

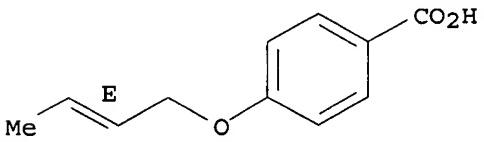


RN 921623-04-3 CAPLUS
CN Benzoic acid, 4-(2,2-difluoroethoxy)- (CA INDEX NAME)

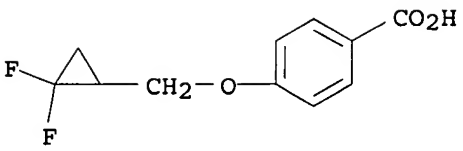


RN 921623-07-6 CAPLUS
CN Benzoic acid, 4-[(2E)-2-buten-1-yloxy]- (CA INDEX NAME)

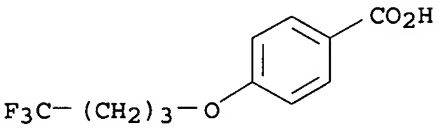
Double bond geometry as shown.



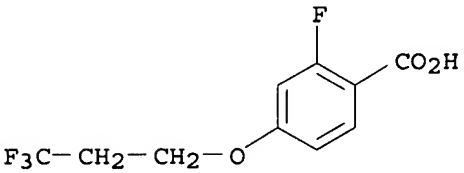
RN 921623-15-6 CAPLUS
CN Benzoic acid, 4-[(2,2-difluorocyclopropyl)methoxy]- (CA INDEX NAME)



RN 921623-31-6 CAPLUS
CN Benzoic acid, 4-(4,4,4-trifluorobutoxy)- (CA INDEX NAME)



RN 921623-34-9 CAPLUS
CN Benzoic acid, 2-fluoro-4-(3,3,3-trifluoropropoxy)- (CA INDEX NAME)



RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:17789 CAPLUS
DN 146:121750
TI Processes for the preparation of protected-(+)-catechin and (-)-epicatechin monomers, for coupling the protected monomers with an activated, protected epicatechin monomer, and for the preparation of epicatechin-(4b,8)-epicatechin or -catechin dimers and their digallates
IN Romanczyk, Leo; Sharma, Pradeep K.; Kolchinski, Alexander G.; Shea, Helene A.; Gou, Yanni
PA USA
SO U.S. Pat. Appl. Publ., 9pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2007004796	A1	20070104	US 2005-169860	20050629
WO 2007005248	A2	20070111	WO 2006-US23698	20060619
WO 2007005248	A3	20070726		

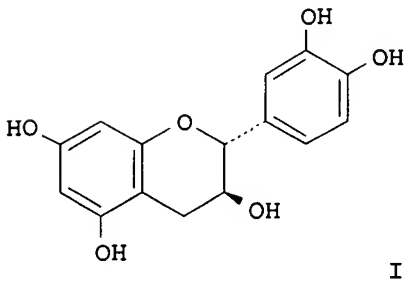
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,

GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

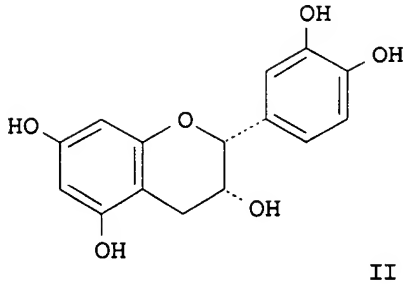
PRAI US 2005-169860 A 20050629

OS CASREACT 146:121750

GI



I



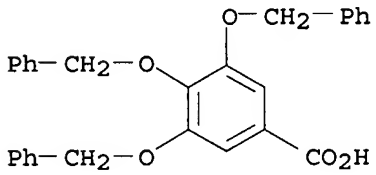
II

AB Improved processes for the preparation of tetra-O-benzyl protected catechin (I), for the coupling of the tetra-O-benzyl protected catechin or epicatechin (II) with a C-4 activated, tetra-O-benzyl protected epicatechin for the galloylation of the epicatechin-(4β,8)-catechin or -epicatechin dimer-the dimer digallates, and for the deprotection (i.e., debenzylation) of the protected epicatechin dimers and protected epicatechin dimer digallates are disclosed.

IT 1486-48-2, Tri-O-benzylgallic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(galloylation by, of protected catechin/epicatechin dimers; preparation of protected-(+)-catechin and (-)-epicatechin monomers, for coupling the with an activated, protected epicatechin monomer)

RN 1486-48-2 CAPLUS

CN Benzoic acid, 3,4,5-tris(phenylmethoxy)- (CA INDEX NAME)



L15 ANSWER 7 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2006:1337786 CAPLUS

DN 146:82154

TI A process for the synthesis of anthocyanins

IN Bakstad, Einar

PA Biosynth A/S, Norway; Beacham, Annabel Rose

SO PCT Int. Appl., 40pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006134352	A1	20061221	WO 2006-GB2172	20060615

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW,

MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI GB 2005-12206 A 20050615

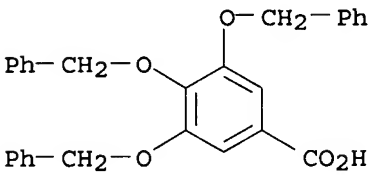
OS MARPAT 146:82154

AB A process for the preparing anthocyanins and precursors of anthocyanins is presented. A coupling reaction between a sugar and a suitable electrophilic precursor to form Eastern half intermediates, that are then reacted with Western half intermediates to form the target anthocyanins is the key step. Some Eastern half intermediates and electrophilic precursors also form part of the invention.

IT 1486-48-2P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for the synthesis of anthocyanins)

RN 1486-48-2 CAPLUS

CN Benzoic acid, 3,4,5-tris(phenylmethoxy)- (CA INDEX NAME)



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 8 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2006:1287282 CAPLUS

DN 147:234506

TI Lawesson's reagent for direct thionation of hydroxamic acids: substituent effects on LR reactivity

AU Przychodzen, Witold

CS Faculty of Chemistry, Gdansk University of Technology, Gdansk, 80-952, Pol.

SO Heteroatom Chemistry (2006), 17(7), 676-684
CODEN: HETCE8; ISSN: 1042-7163

PB John Wiley & Sons, Inc.

DT Journal

LA English

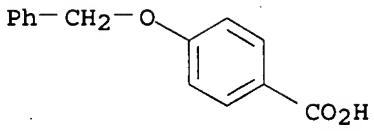
OS CASREACT 147:234506

AB To explore the generality and scope of direct thionation of hydroxamic acids (HAs), the reaction of various structurally diverse HAs with Lawesson's reagent was investigated. The yield of thiohydroxamic acid (THAs) is poor when HAs possess bulky acyl and/or N-substituents, acidic α-hydrogen atoms, or an N-Ph ring. THAs yields were correlated with Brown sigma parameter. The relative rates of two subsequent processes kT2 and kR2 were also measured. Correlation was also found for methine proton chemical shifts of N-iso-Pr benzothiohydroxamic acids.

IT 1486-51-7, 4-Benzyloxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(substituent effect and reactivity of Lawesson's reagent for direct thionation of hydroxamic acids)

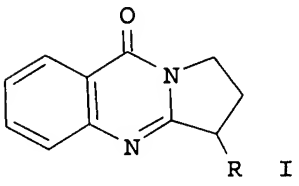
RN 1486-51-7 CAPLUS

CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)

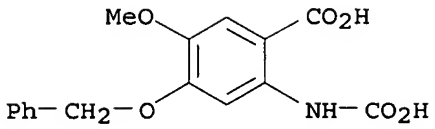


RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

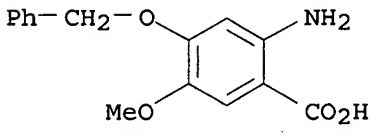
L15 ANSWER 9 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1245430 CAPLUS
DN 146:163292
TI Solid-phase synthesis of fused [2,1-b]quinazolinone alkaloids
AU Kamal, Ahmed; Shankaraiah, N.; Devaiah, V.; Reddy, K. Laxma
CS Biotransformation Laboratory, Division of Organic Chemistry, Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SO Tetrahedron Letters (2006), 47(51), 9025-9028
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Ltd.
DT Journal
LA English
OS CASREACT 146:163292
GI



AB Solid-phase synthesis of fused [2,1-b]quinazolinone alkaloids has been developed for the preparation of vasicinone (I; R = OH) and deoxyvasicinone (I; R = H) by two approaches. The derivative of polymer-supported p-nitrophenyl carbonate was attached to anthranilic acid and then coupled with various bromo-lactams. This resin-linked bromo intermediate upon acetylation, hydrolysis and resin cleavage gave the cyclized [2,1-b]quinazolinones (vasicinone). Alternatively, resin-linked azido-benzoic acids were coupled with bromo-substituted lactams followed by cyclization in an aza-Wittig reductive cyclization process giving the bromo-substituted quinazolinone intermediates, with subsequent acetylation, hydrolysis and resin cleavage affording the fused [2,1-b]quinazolinones.
IT 919511-98-1DP, resin-bound urethane
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of, by lactams; solid-phase synthesis of fused [2,1-b]quinazolinone alkaloids)
RN 919511-98-1 CAPLUS
CN Benzoic acid, 2-(carboxyamino)-5-methoxy-4-(phenylmethoxy)- (CA INDEX NAME)



IT 155666-33-4, 4-Benzyloxy-5-methoxyanthranilic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Wang resin nitrophenyl carbonate; solid-phase synthesis of fused [2,1-b]quinazolinone alkaloids)
RN 155666-33-4 CAPLUS
CN Benzoic acid, 2-amino-5-methoxy-4-(phenylmethoxy)- (CA INDEX NAME)



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 10 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1120609 CAPLUS
DN 145:438648
TI Preparation of heterocyclic sulfamate compounds as inhibitors of estrone sulfatase and aromatase for treating cancer
IN Reed, Michael John; Potter, Barry Victor Lloyd
PA Sterix Ltd., UK
SO U.S. Pat. Appl. Publ., 95pp., Cont.-in-part of U.S. Ser. No. 991,137.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 14

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2006241173	A1	20061026	US 2006-400791	20060407
WO 9730041	A1	19970821	WO 1997-GB444	19970217
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RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
EP 1577308	A2	20050921	EP 2005-983	19970217
EP 1577308	A3	20070829		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, FI				
CN 1701790	A	20051130	CN 2005-10075895	19970217
CN 1989961	A	20070704	CN 2006-10101905	19970217
WO 9732872	A1	19970912	WO 1997-GB600	19970304
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU				
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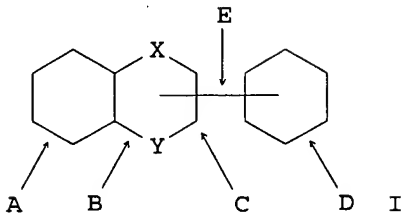
EP 1502915	A1	20050202	EP 2004-25526	19970304
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, FI				
US 6011024	A	20000104	US 1998-111927	19980708

	US 6239169	B1	20010529	US 1998-125255	19980814
	US 6187766	B1	20010213	US 1999-238345	19990127
	AU 726811	B2	20001123	AU 2000-10130	20000106
	US 6506792	B1	20030114	US 2000-638315	20000814
	US 6921776	B1	20050726	US 2000-638314	20000814
	AU 769753	B2	20040205	AU 2001-23181	20010222
	US 2003162752	A1	20030828	US 2002-327500	20021220
	US 7129269	B2	20061031		
	US 2005154050	A1	20050714	US 2004-991137	20041117
	US 7202272	B2	20070410		

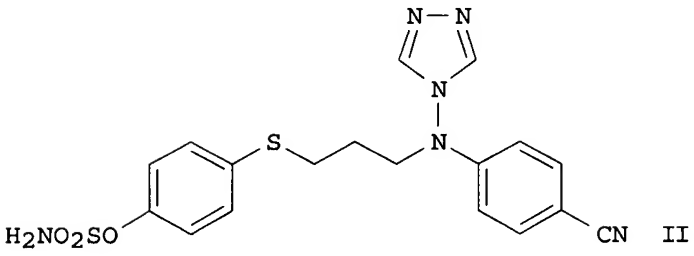
PRAI GB 1996-3325 A 19960216
GB 1996-4709 A 19960305
GB 1996-5725 A 19960319
WO 1997-GB444 A2 19970217
WO 1997-GB600 A2 19970304
US 1998-111927 A3 19980708
US 1998-125255 A2 19980814
US 1999-238345 A2 19990127
US 2000-638314 A3 20000814
US 2000-638315 A3 20000814
US 2002-327500 A2 20021220
US 2004-991137 A2 20041117
GB 1991-18478 A 19910829
US 1994-196192 A3 19941227
US 1995-458352 A2 19950602
CN 1997-193826 A3 19970217
CN 2005-10075895 A3 19970217
EP 1997-903494 A3 19970821
EP 1997-905332 A3 19970912
WO 1997-GB3352 A2 19971204
AU 1999-10077 A 19990111
AU 2000-10130 A3 20000106

OS MARPAT 145:438648

GI



I



II

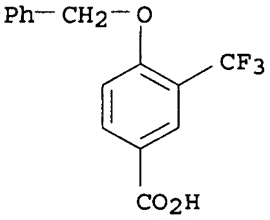
AB The present invention relates to sulfamate compds. that are an inhibitor of both estrone sulfatase activity and aromatase activity. Among the general structures that the sulfamate compound may have is I, wherein A represents the first ring structure, B represents the third ring structure, D represents the second ring structure, C is an optional double bond, E is a link joining the second ring structure to the third ring

structure, X represents a suitable first group, and Y represents a suitable second group; wherein any one of ring structures A, B and D is a phenolic ring; and wherein any one of ring structures A, B and D has bound thereto a sulfamate group. The present invention provides compds. that have considerable therapeutic advantages, particularly for treating breast and endometrial cancers. Pharmaceutical compns. comprising the sulfamates of the invention, as well as a process for preparing same. For example, II was prepared by reaction of 4-[[3-(4-hydroxyphenylsulfanyl)propyl]-[1,2,4]triazol-4-ylamino]benzonitrile (prepared in 2 steps from 4-([1,2,4]triazol-4-ylamino)benzonitrile and 1,3-dibromopropane) with sulfamoyl chloride. II (10 mg/kg, orally) decreased estradiol levels by 82% in rats treated with pregnant mare serum gonadotropin to induced estrogen synthesis.

IT 536975-35-6P, 4-Benzyloxy-3-trifluoromethylbenzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclic sulfamate compds. as inhibitors of estrone sulfatase and aromatase for treating cancer)

RN 536975-35-6 CAPLUS

CN Benzoic acid, 4-(phenylmethoxy)-3-(trifluoromethyl)- (CA INDEX NAME)



L15 ANSWER 11 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2006:1033643 CAPLUS

DN 145:397502

TI Preparation of oxazoline and thiazoline derivatives as histamine H3-receptor ligands with numerous therapeutic uses

IN Celanire, Sylvain; Talaga, Patrice; Leurs, Regorius; Denonne, Frederic; Timmerman, Henkdrik; Lebon, Florence

PA Ucb S.A., Belg.

SO PCT Int. Appl., 106pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006103057	A1	20061005	WO 2006-EP2860	20060329

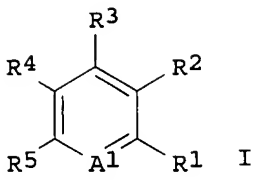
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI EP 2005-6971 A 20050331

OS MARPAT 145:397502

GI



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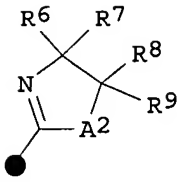


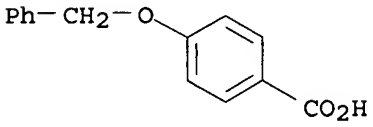
II

AB The present invention relates to compds. comprising an oxazoline or thiazoline moiety (shown as I; variables defined below; e.g. 1-[3-[4-(4,4-dimethyl-4,5-dihydro-1,3-oxazol-2-yl)phenoxy]propyl]piperidine (1)), processes for preparing them (synthetic intermediates but no methods of preparation are claimed), pharmaceutical compns. comprising said compds. and their uses (no data) as H3-receptor ligands. For I: A1 is CH, CMe or N; R1 is H or halogen; R2 is II; A2 is O or S; R3 is H, halogen, C1-4 alkyl or C1-4 alkoxy; R4 is H, halogen, C1-4 alkyl, C1-4 alkoxy, trifluoromethyl or -O(CH2)nNR12aR12b each CH2 in -O(CH2)nNR12aR12b being (un)substituted by one or two C1-4 alkyl; R5 is H or -O(CH2)mNR13aR13b, each CH2 in -O(CH2)mNR13aR13b being (un)substituted by one or two C1-4 alkyl, and at least one of R4 and R5 should be a -O(CH2)nNR12a/13aR12b/13b group; addnl. details including provisos are given in the claims. Although the methods of preparation are not claimed, prepns. and/or characterization data for >30 examples of I are included. For example, 1 was prepared in 5 steps (80, 99, 95, 97 and 83 %) starting from 4-benzyloxybenzoic acid and 2-amino-2-methylpropan-1-ol to give 4-(benzyloxy)-N-(2-hydroxy-1,1-dimethylethyl)benzamide, with subsequent formation of the following intermediates: 2-[4-(benzyloxy)phenyl]-4,4-dimethyl-4,5-dihydro-1,3-oxazole, 4-(4,4-dimethyl-4,5-dihydro-1,3-oxazol-2-yl)phenol and 2-[4-(3-chloropropoxy)phenyl]-4,4-dimethyl-4,5-dihydro-1,3-oxazole. In an [35S]GTPγS-binding assay using human histamine H3-receptor, compds. I showed pIC50 6.5-10. In a paced isolated guinea pig myenteric plexus - elec.-field stimulation assay for antagonism activity, compds. I showed pA2 values typically ≥6.5 for the histamine H3 receptor.

IT 1486-51-7, 4-Benzyloxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of oxazoline and thiazoline derivs. as histamine H3-receptor ligands with numerous therapeutic uses)

RN 1486-51-7 CAPLUS

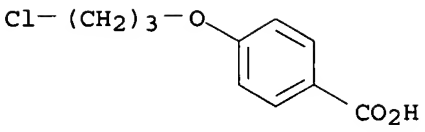
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



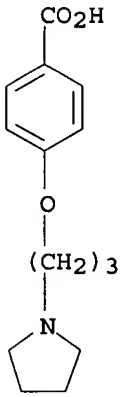
IT 65136-52-9P, 4-(3-Chloropropoxy)benzoic acid 764629-16-5P, 4-[3-(Pyrrolidin-1-yl)propoxy]benzoic acid 767286-87-3P, 4-[3-(Piperidin-1-yl)propoxy]benzoic acid 911198-63-5P, 4-[3-(2-Methylpiperidin-1-yl)propoxy]benzoic acid 911198-64-6P, 4-[3-(2,6-Dimethylpiperidin-1-yl)propoxy]benzoic acid 911198-65-7P, 4-[3-(2-Methylpyrrolidin-1-yl)propoxy]benzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of oxazoline and thiazoline derivs. as histamine H3-receptor ligands with numerous therapeutic uses)

RN 65136-52-9 CAPLUS

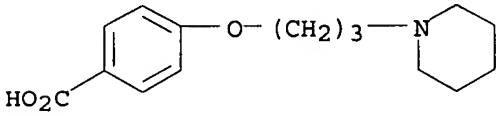
CN Benzoic acid, 4-(3-chloropropoxy)- (9CI) (CA INDEX NAME)



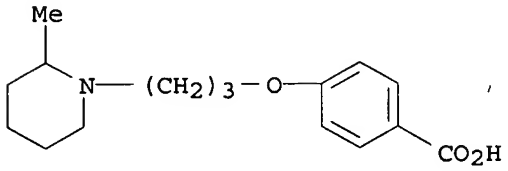
RN 764629-16-5 CAPLUS
CN Benzoic acid, 4-[3-(1-pyrrolidinyl)propoxy]- (9CI) (CA INDEX NAME)



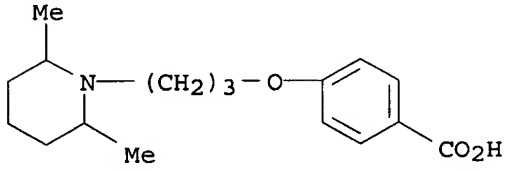
RN 767286-87-3 CAPLUS
CN Benzoic acid, 4-[3-(1-piperidinyl)propoxy]- (9CI) (CA INDEX NAME)



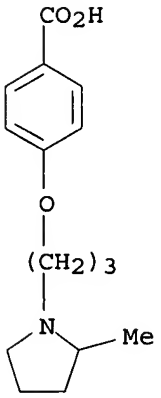
RN 911198-63-5 CAPLUS
CN Benzoic acid, 4-[3-(2-methyl-1-piperidinyl)propoxy]- (CA INDEX NAME)



RN 911198-64-6 CAPLUS
CN Benzoic acid, 4-[3-(2,6-dimethyl-1-piperidinyl)propoxy]- (CA INDEX NAME)



RN 911198-65-7 CAPLUS
CN Benzoic acid, 4-[3-(2-methyl-1-pyrrolidinyl)propoxy]- (CA INDEX NAME)



RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

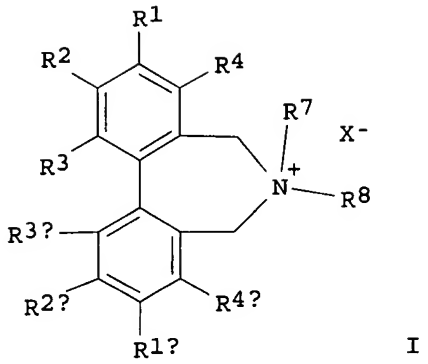
L15 ANSWER 12 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1031261 CAPLUS
DN 145:419469
TI Preparation of optically active quaternary ammonium salts having axial asymmetry and process for producing α-amino acids and derivatives thereof using said quaternary ammonium salts as phase transfer catalysts
IN Maruoka, Keiji; Nishimoto, Yukifumi; Yamamoto, Kenichiro
PA Nagase & Co., Ltd., Japan; Kyoto University
SO PCT Int. Appl., 374pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006104226	A1	20061005	WO 2006-JP306791	20060324

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI JP 2005-94873 A 20050329
OS MARPAT 145:419469
GI



I

AB The title quaternary ammonium salts I [R1, R1a, R2, R2a = H, halo, (un)substituted alkyl, etc.; R3, R3a = halo, (un)substituted alkyl, (un)substituted alkoxy; R4, R4a = H, cyano, nitro, etc.; R7, R8 = (halo)alkyl, (halo)alkenyl, (halo)alkynyl, etc.; X- = SCN-, HSO4-, etc.] are prepared The preparation of α-amino acids using said quaternary ammonium salts as phase transfer catalysts is disclosed. Thus, reaction of N-(diphenylmethylene)glycine tert-Bu ester with benzyl bromide in a mixture of aqueous KOH and toluene containing an optically active quaternary ammonium salt of this invention gave (R)-tert-Bu N-(diphenylmethylene)phenylalanine (98% ee) in 95% yield.

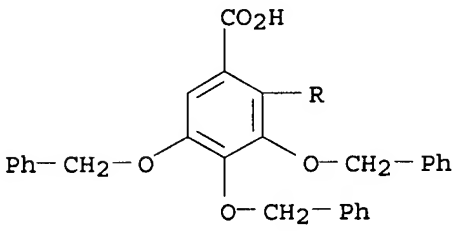
IT 911701-74-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(optically active, unspecified; preparation of optically active quaternary ammonium salts having axial asymmetry and process for producing α-amino acids and derivs. thereof using said quaternary ammonium salts as phase transfer catalysts)

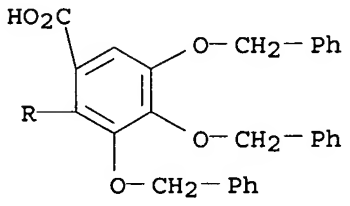
RN 911701-74-1 CAPLUS

CN Cinchonan-9-ol, 6'-methoxy-, (9S)-, 4,4',5,5',6,6'-hexakis(phenylmethoxy)[1,1'-biphenyl]-2,2'-dicarboxylate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 97152-40-4
CMF C56 H46 O10

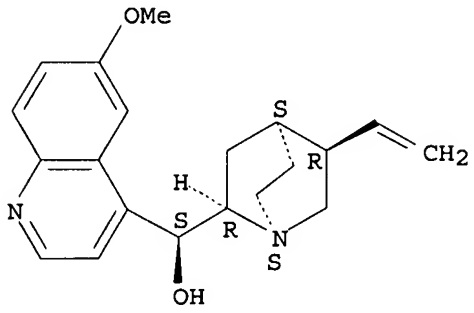




CM 2

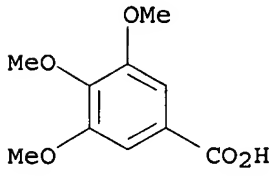
CRN 56-54-2
CMF C20 H24 N2 O2

Absolute stereochemistry. Rotation (+).

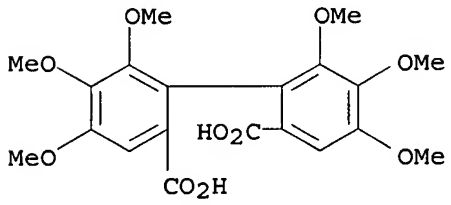


IT 118-41-2, reactions 2292-39-9 6970-19-0
21553-46-8 133358-96-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of optically active quaternary ammonium salts having axial asymmetry and process for producing α-amino acids and derivs. thereof using said quaternary ammonium salts as phase transfer catalysts)

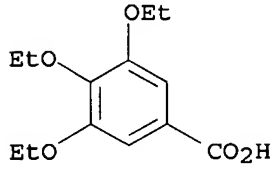
RN 118-41-2 CAPLUS
CN Benzoic acid, 3,4,5-trimethoxy- (CA INDEX NAME)



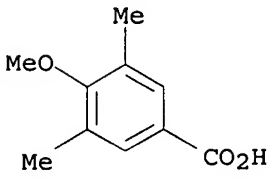
RN 2292-39-9 CAPLUS
CN [1,1'-Biphenyl]-2,2'-dicarboxylic acid, 4,4',5,5',6,6'-hexamethoxy- (9CI) (CA INDEX NAME)



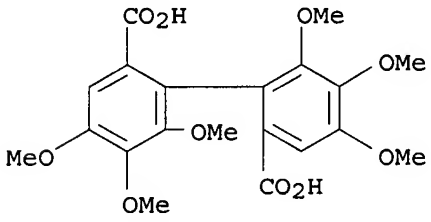
RN 6970-19-0 CAPLUS
CN Benzoic acid, 3,4,5-triethoxy- (CA INDEX NAME)



RN 21553-46-8 CAPLUS
CN Benzoic acid, 4-methoxy-3,5-dimethyl- (9CI) (CA INDEX NAME)

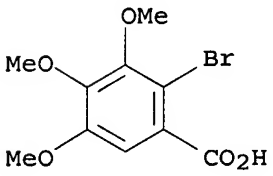


RN 133358-96-0 CAPLUS
CN [1,1'-Biphenyl]-2,2'-dicarboxylic acid, 4,4',5,5',6,6'-hexamethoxy-, (1S)-(9CI) (CA INDEX NAME)

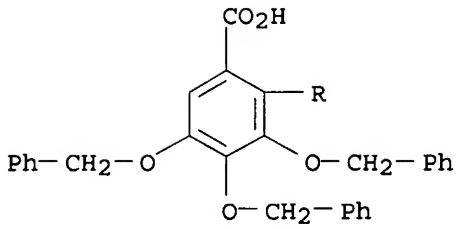


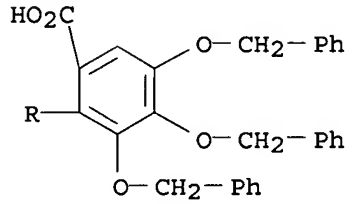
IT 23346-82-9P 97152-40-4P 105175-61-9P
124854-06-4P 195884-87-8P 911701-67-2P
911701-69-4P 911701-82-1P 911822-70-3P
911822-78-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active quaternary ammonium salts having axial asymmetry and process for producing α-amino acids and derivs. thereof using said quaternary ammonium salts as phase transfer catalysts)

RN 23346-82-9 CAPLUS
CN Benzoic acid, 2-bromo-3,4,5-trimethoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)

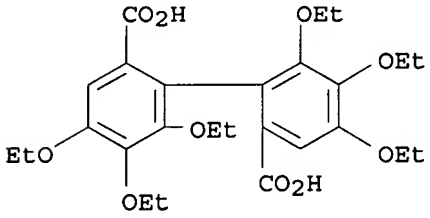


RN 97152-40-4 CAPLUS
CN [1,1'-Biphenyl]-2,2'-dicarboxylic acid, 4,4',5,5',6,6'-hexakis(phenylmethoxy)- (9CI) (CA INDEX NAME)

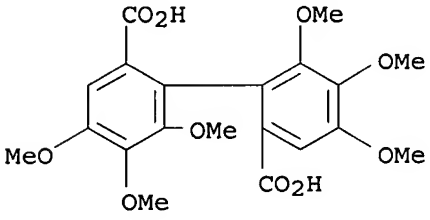




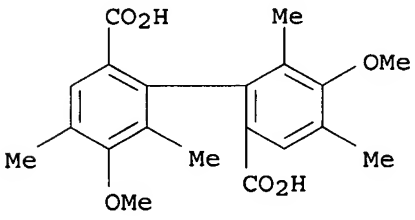
RN 105175-61-9 CAPLUS
CN [1,1'-Biphenyl]-2,2'-dicarboxylic acid, 4,4',5,5',6,6'-hexaethoxy- (9CI) (CA INDEX NAME)



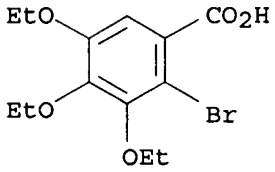
RN 124854-06-4 CAPLUS
CN [1,1'-Biphenyl]-2,2'-dicarboxylic acid, 4,4',5,5',6,6'-hexamethoxy-, (1R)- (9CI) (CA INDEX NAME)



RN 195884-87-8 CAPLUS
CN [1,1'-Biphenyl]-2,2'-dicarboxylic acid, 5,5'-dimethoxy-4,4',6,6'-tetramethyl- (9CI) (CA INDEX NAME)



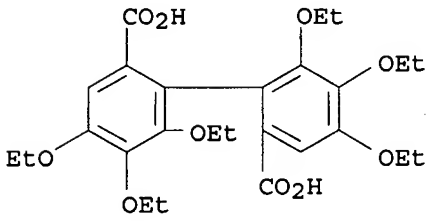
RN 911701-67-2 CAPLUS
CN Benzoic acid, 2-bromo-3,4,5-triethoxy- (CA INDEX NAME)



RN 911701-69-4 CAPLUS
CN Cinchonan-9-ol, 6'-methoxy-, (9S)-, 4,4',5,5',6,6'-hexaethoxy[1,1'-biphenyl]-2,2'-dicarboxylate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

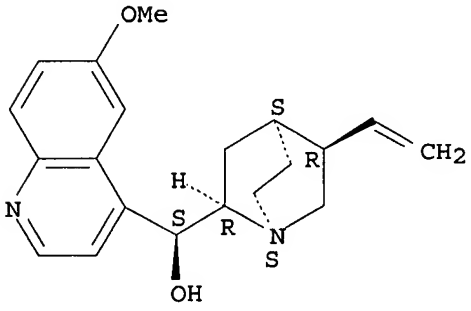
CRN 105175-61-9
CMF C26 H34 O10



CM 2

CRN 56-54-2
CMF C20 H24 N2 O2

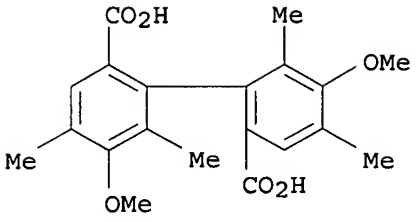
Absolute stereochemistry. Rotation (+).



RN 911701-82-1 CAPLUS
CN Cinchonan-9-ol, 6'-methoxy-, (9S)-, 5,5'-dimethoxy-4,4',6,6'-tetramethyl[1,1'-biphenyl]-2,2'-dicarboxylate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

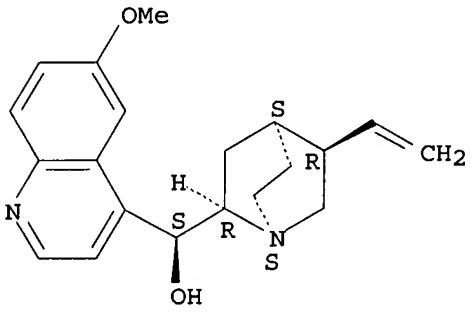
CRN 195884-87-8
CMF C20 H22 O6



CM 2

CRN 56-54-2
CMF C20 H24 N2 O2

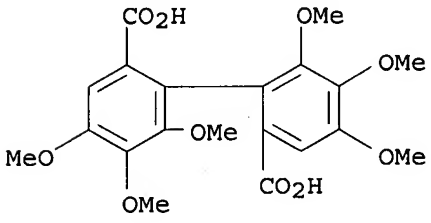
Absolute stereochemistry. Rotation (+).



RN 911822-70-3 CAPLUS
CN Cinchonan-9-ol, 6'-methoxy-, (9S)-, (R)-4,4',5,5',6,6'-hexamethoxy[1,1'-biphenyl]-2,2'-dicarboxylate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

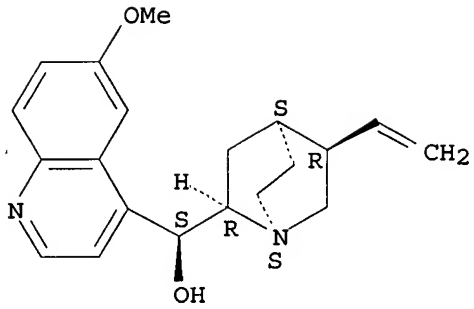
CRN 124854-06-4
CMF C20 H22 O10



CM 2

CRN 56-54-2
CMF C20 H24 N2 O2

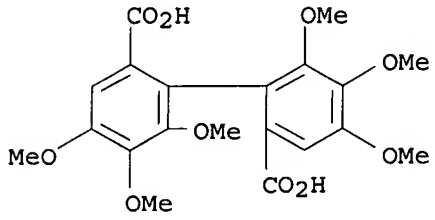
Absolute stereochemistry. Rotation (+).



RN 911822-78-1 CAPLUS
CN Cinchonan-9-ol, 6'-methoxy-, (9S)-, (1S)-4,4',5,5',6,6'-hexamethoxy[1,1'-biphenyl]-2,2'-dicarboxylate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

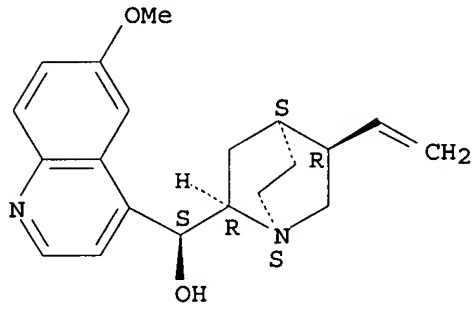
CRN 133358-96-0
CMF C20 H22 O10



CM 2

CRN 56-54-2
CMF C20 H24 N2 O2

Absolute stereochemistry. Rotation (+).



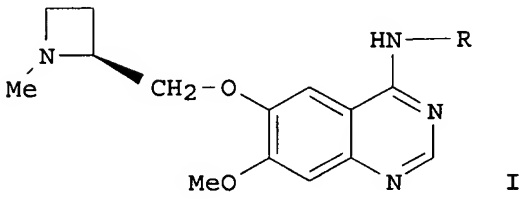
RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 13 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:792977 CAPLUS
DN 145:211063
TI Preparation of quinazoline compounds as antitumor agents
IN Sun, Piaoyang
PA Peop. Rep. China
SO PCT Int. Appl., 36pp.

CODEN: PIXXD2
DT Patent
LA Chinese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006081741	A1	20060810	WO 2006-CN96	20060120
CN 101003513	A	20070725	CN 2006-10001544	20060120

PI WO 2006081741 A1 20060810 WO 2006-CN96 20060120
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
CN 101003513 A 20070725 CN 2006-10001544 20060120
PRAI CN 2005-10037789 A 20050205
OS MARPAT 145:211063
GI

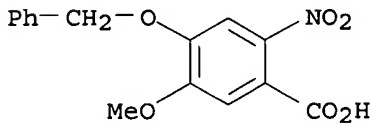


I

AB Title quinazolines e.g. I (R = 3-ethynylphenyl, 3-chloro-4-fluorophenyl) are prepared It also relates to preparation process and medical compns. containing the effective dosage of compds. of title compds. or their salts. It is found that title compds or their salts can treat cellular proliferative disease such as cancer by inhibiting epidermal growth factor receptor protein of cell surface.

IT 60547-92-4P, 4-Benzyloxy-5-methoxy-2-nitrobenzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinazoline compds. as antitumor agents)

RN 60547-92-4 CAPLUS
CN Benzoic acid, 5-methoxy-2-nitro-4-(phenylmethoxy)- (CA INDEX NAME)



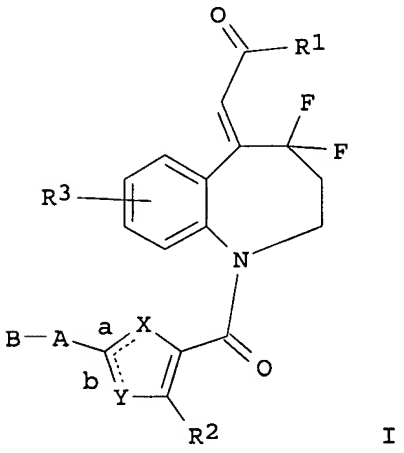
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 14 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:578220 CAPLUS
DN 145:62797
TI Preparation of benzazepine derivatives as vasopressin V2 receptor stimulants
IN Koshio, Hiroyuki; Tsukamoto, Kazunari; Kakefuda, Akio; Akamatsu, Seijiro;

Saito, Shin
PA Astellas Pharma Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 55 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

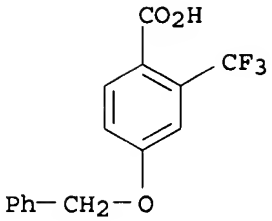
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2006151957	A	20060615	JP 2005-309218	20051025
PRAI JP 2004-311914	A	20041027		

OS MARPAT 145:62797
GI

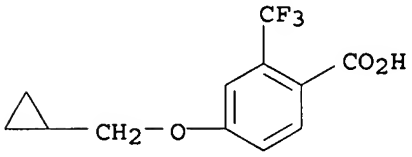


I

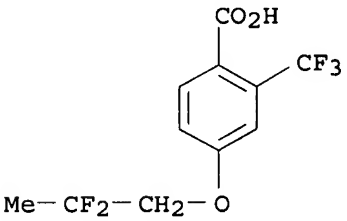
AB The title compds. I [R1 = (un)substituted amino; R2 = CF3, halo; R3 = H, halo; the dotted lines a and b indicate single bond or double bond : one of them is a single bond, the other is a double bond; when a is a single bond and b is a double bond, X = CH:CH, CH:N, S, etc.; when a is a double bond, b is a single bond, X = N; when a is a single bond and b is a double bond, Y = CH, N; when a is a double bond, b is a single bond, Y = S; A = O, S, NH, etc.; B = (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, etc.] are prepared by reaction of I [R1 = OH; others = as defined above] or reactive derivs. thereof with HR1 [R1 = (un)substituted amino]. I are said to be useful in the treatment of nycturia and diabetes insipidus. Thus, (2Z)-N-(2-amino-2-oxoethyl)-2-(1-[4-(benzyloxy)-2-(trifluoromethyl)benzoyl]-4,4-difluoro-1,2,3,4-tetrahydro-5-H-1-benzazepin-5-ylidene)acetamide was prepared in a multistep process starting from benzyl alc. and 4-fluoro-2-trifluoromethylbenzoic acid. In a V2 receptor binding assay, compds. of this invention showed Ki values of 4.3 nM to 19 nM.
IT 790695-23-7P 790695-25-9P 790695-52-2P
790695-56-6P 790695-61-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzazepine derivs. as vasopressin V2 receptor stimulants)
RN 790695-23-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 790695-25-9 CAPLUS
CN Benzoic acid, 4-(cyclopropylmethoxy)-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

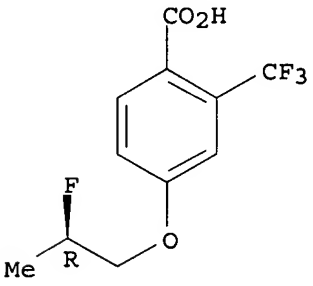


RN 790695-52-2 CAPLUS
CN Benzoic acid, 4-(2,2-difluoropropoxy)-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



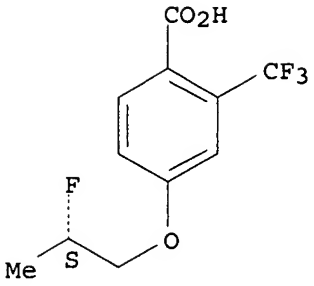
RN 790695-56-6 CAPLUS
CN Benzoic acid, 4-[(2R)-2-fluoropropoxy]-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 790695-61-3 CAPLUS
CN Benzoic acid, 4-[(2S)-2-fluoropropoxy]-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 15 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:493830 CAPLUS
DN 145:8166
TI Preparation of benzimidazoles as gonadotropin releasing hormone receptor antagonists for treating disorders associated with excessive GnRH receptor activity
IN Garrick, Lloyd Michael; Green, Daniel Michael; Jetter, James Winfield; Kao, Wenling; Kees, Kenneth Lewis; Pelletier, Jeffrey Claude; Rogers, John Francis
PA Wyeth, John, and Brother Ltd., USA
SO U.S. Pat. Appl. Publ., 72 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2006111355	A1	20060525	US 2005-286081	20051123
	AU 2005309647	A1	20060601	AU 2005-309647	20051121
	CA 2587853	A1	20060601	CA 2005-2587853	20051121
	WO 2006058012	A2	20060601	WO 2005-US42338	20051121
	WO 2006058012	A3	20061005		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	EP 1814866	A2	20070808	EP 2005-825094	20051121
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
	IN 2007DN03796	A	20070824	IN 2007-DN3796	20070522
PRAI	US 2004-630282P	P	20041123		
	WO 2005-US42338	W	20051121		

OS MARPAT 145:8166
GI

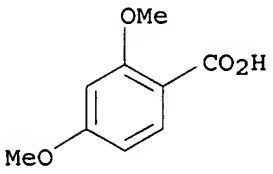
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to gonadotropin releasing hormone (GnRH) (also known as LH releasing hormone) receptor antagonists, processes for preparing them and to pharmaceutical compns. containing

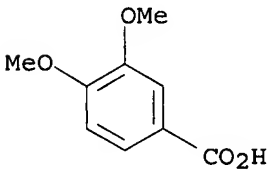
them. The antagonists are of general formula I wherein: A is cycloalkyl, aryl, heteroaryl, or diaryl substituted alkyl, each optionally substituted; B is aryl or heteroaryl, each optionally substituted; R1 is H, the tautomeric form, or optionally substituted alkyl; R2, R3, and R4 are, independently, H, optionally substituted alkyl, halogen, or OR1; and R5, R6, R7, R8, R9, R10, R11, R12, R13, R14, R15, and R16, are, independently, H, alkyl, alkenyl, or alkynyl, each alkyl, alkenyl, or alkynyl being optionally substituted. For example, II was prepared by reacting 4-(Dimethylamino)benzoic acid with the appropriate phenylenediamine (preparation given). All I tested in an in vitro assay involving COS cell membranes containing human GnRH receptors had IC50's between 1 and 10,000 nM.

IT 91-52-1 93-07-2 100-09-4 330-12-1
570-02-5 619-86-3 645-08-9 1142-39-8
1486-51-7 1498-96-0 5438-19-7
15872-41-0 15872-42-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzimidazoles as gonadotropin releasing hormone receptor antagonists for treating disorders associated with excessive GnRH receptor activity)

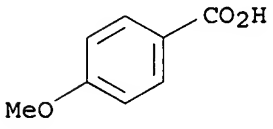
RN 91-52-1 CAPLUS
CN Benzoic acid, 2,4-dimethoxy- (CA INDEX NAME)



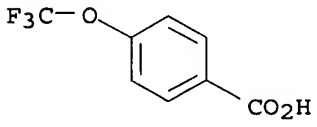
RN 93-07-2 CAPLUS
CN Benzoic acid, 3,4-dimethoxy- (CA INDEX NAME)



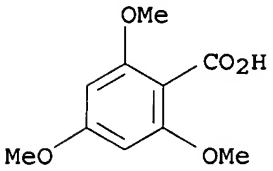
RN 100-09-4 CAPLUS
CN Benzoic acid, 4-methoxy- (CA INDEX NAME)



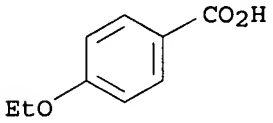
RN 330-12-1 CAPLUS
CN Benzoic acid, 4-(trifluoromethoxy)- (CA INDEX NAME)



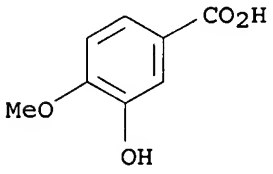
RN 570-02-5 CAPLUS
CN Benzoic acid, 2,4,6-trimethoxy- (CA INDEX NAME)



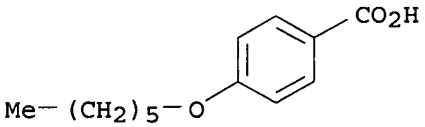
RN 619-86-3 CAPLUS
CN Benzoic acid, 4-ethoxy- (CA INDEX NAME)



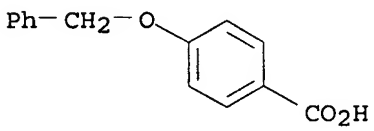
RN 645-08-9 CAPLUS
CN Benzoic acid, 3-hydroxy-4-methoxy- (CA INDEX NAME)



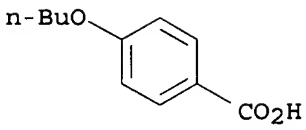
RN 1142-39-8 CAPLUS
CN Benzoic acid, 4-(hexyloxy)- (CA INDEX NAME)



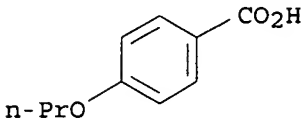
RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



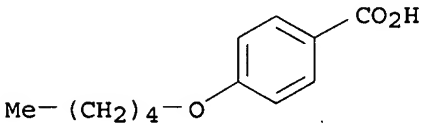
RN 1498-96-0 CAPLUS
CN Benzoic acid, 4-butoxy- (CA INDEX NAME)



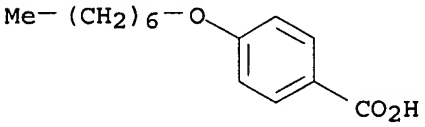
RN 5438-19-7 CAPLUS
CN Benzoic acid, 4-propoxy- (CA INDEX NAME)



RN 15872-41-0 CAPLUS
CN Benzoic acid, 4-(pentyloxy)- (CA INDEX NAME)



RN 15872-42-1 CAPLUS
CN Benzoic acid, 4-(heptyloxy)- (CA INDEX NAME)



L15 ANSWER 16 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:362641 CAPLUS
DN 144:350688
TI Losartan derivatives with antioxidant properties, and their preparation and use as antihypertensives with tissue damage prevention activities
IN Alajarin Ferrandez, Ramon; Alvarez-Builla Gomez, Julio; Diez Marques, Maria Luisa; Garcia Navazo, Gonzalo; Rodriguez Puyol, Diego; Rodriguez Puyol, Manuel
PA Universidad de Alcala, Spain
SO Span., 19 pp.
CODEN: SPXXAD
DT Patent
LA Spanish
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	ES 2242543	A1	20051101	ES 2004-1050	20040430
	ES 2242543	B1	20061201		
PRAI	ES 2004-1050		20040430		

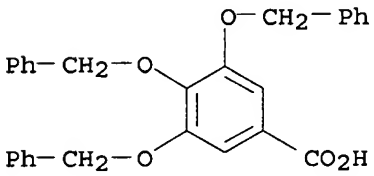
OS CASREACT 144:350688; MARPAT 144:350688
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

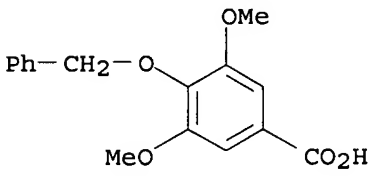
AB Losartan derivs. I and a process for their preparation are disclosed [in which: X = H, Cl; A = residue of 8 specific phenolic carboxylic acid antioxidants, e.g., 3,4-dihydroxybenzoyl]. The preparation process involves Mitsunobu reaction of tritylated losartan derivative II with corresponding, optionally protected antioxidant acids, followed by appropriate deprotection of the obtained intermediate. Depending upon the deprotective conditions, the chlorine atom of II may or may not remain. I are prepared as pharmaceuticals with simultaneous angiotensin II receptor-blocking and antioxidant properties, and are beneficial for preventing tissue damage in patients with cardiovascular risks. Thus, Mitsunobu reaction of II with 3-[3,4-bis(benzyloxy)phenyl]propanioic acid in the presence of PPh3 and di-Me azodicarboxylate in Et2O gave 63% intermediate III. Hydrogenolytic deprotection of III with 1 atm H2 over 30% Pd/C, with concomitant dechlorination, gave 56% invention compound IV, designated GGN 841. In tests for displacement of labeled angiotensin II from its receptor, and for inhibition of angiotensin II-induced contraction of human mesangial cells in vitro, IV was as active or slightly more active than losartan itself. In addition, the antioxidant activity of IV, determined by inhibition of the oxidation of ABTS in vitro, was 8-fold greater than that of losartan.

IT 1486-48-2, 3,4,5-Tris(benzyloxy)benzoic acid 14588-60-4, 4-(Benzyloxy)-3,5-dimethoxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; losartan derivs. with antioxidant properties, and their preparation and use as antihypertensives with tissue damage prevention activities)

RN 1486-48-2 CAPLUS
CN Benzoic acid, 3,4,5-tris(phenylmethoxy)- (CA INDEX NAME)



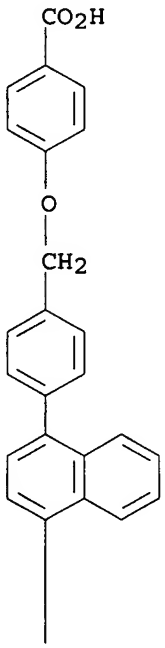
RN 14588-60-4 CAPLUS
CN Benzoic acid, 3,5-dimethoxy-4-(phenylmethoxy)- (CA INDEX NAME)

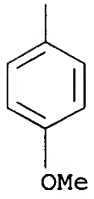


L15 ANSWER 17 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:93715 CAPLUS
DN 144:421562
TI Sensitized emission of luminescent lanthanide complexes based on 4-naphthalen-1-yl-benzoic acid derivatives by a charge-transfer process
AU Kim, Yong Hee; Baek, Nam Seob; Kim, Hwan Kyu
CS Center for Smart Light-Harvesting Materials & Department of Polymer Science & Engineering, Hannam University, Daejeon, 306-791, S. Korea
SO ChemPhysChem (2006), 7(1), 213-221
CODEN: CPCHFT; ISSN: 1439-4235

PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
AB The photophys. properties of 4-naphthalen-1-ylbenzoic acid ligands and their EuIII-cored complexes were systematically studied to elucidate the effective energy transfer pathway in luminescent lanthanide complexes. 4-Naphthalen-1-ylbenzoic acid ligands, such as 4-naphthalen-1-ylbenzoic acid (NA-1), 4-[4-(4-methoxyphenyl)naphthalen-1-yl]benzoic acid (NA-2), and 4-{4-[4-(4-methoxyphenyl)naphthalen-1-yl]benzyloxy}benzoic acid (NA-3), were synthesized and used for the synthesis of their EuIII-cored complexes, corresponding to NAC-1, NAC-2, and NAC-3. The fluorescence of NA-1 and NA-2 show large Stokes shifts with increasing solvent polarity. These large Stokes shifts might be dominantly due to the formation of an intramol. charge transfer (ICT) complex in the excited state. The intensive luminescence of EuIII by the photoexcitation of the ligand in NAC-1 and NAC-2 in polar solvents supports that the energy transfer from the ligand to the EuIII ion takes place efficiently. In the case of NA-3, which has a -CH2OPh- group that acts as a blocking group, there is no dependence of the fluorescence on the solvent nature and no luminescence of the EuIII ions by the photoexcitation of the ligand, indicating no formation of the ICT state. This can be due to the fact that the formation of the ICT state in NA-3 was prevented because the -OCH2- group acts as a blocking group by interrupting the π-conjugation between the HOBz and the naphthalene unit. From these photophys. studies, probably the ICT state plays a very important role in the energy-transfer pathway from the ligand to the EuIII ion. To the best knowledge, this is the 1st demonstration of sensitized emission of luminescent lanthanide complexes based on 4-naphthalen-1-ylbenzoic acid derivs. by the charge-transfer process.
IT 883877-10-9
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(sensitized emission by charge-transfer process in)
RN 883877-10-9 CAPLUS
CN Benzoic acid, 4-[[4-[4-(4-methoxyphenyl)-1-naphthalenyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

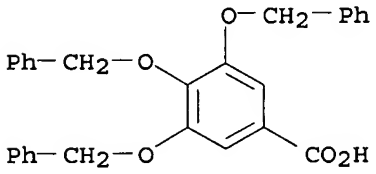
PAGE 1-A



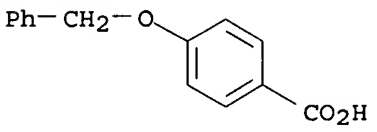


RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 18 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:14204 CAPLUS
DN 145:98462
TI A structure-activity study for the inhibition of metalloproteinase-9 activity and gene expression by analogues of gallocatechin-3-gallate
AU Dell'Agli, M.; Bellosta, S.; Rizzi, L.; Galli, G. V.; Canavesi, M.; Rota, F.; Parente, R.; Bosisio, E.; Romeo, S.
CS Department of Pharmacological Sciences, University of Milan, Milan, 20133, Italy
SO Cellular and Molecular Life Sciences (2005), 62(23), 2896-2903
CODEN: CMLSFI; ISSN: 1420-682X
PB Birkhaeuser Verlag
DT Journal
LA English
OS CASREACT 145:98462
AB Catechins are able to modulate the gelatinolytic activity of matrix metalloproteinase-9 (MMP-9) by reducing its release from macrophages. Gallocatechins decrease MMP-9 secretion by lowering MMP-9 promoter activity and mRNA levels. The effect appears to be dependent on some structural and stereochem. requirements. In this study, the relationship between chemical structure and activity was studied by testing the effect of analogs of (±)-gallocatechin-3-gallate (±)-GCG, selectively deprived of hydroxyl groups, on MMP-9 activity, transcription, and secretion. Our results indicate that (±)-GCG and (±)-catechin-3-gallate are characterized by a substitution pattern compatible with direct inhibition of MMP-9 activity. Conversely, when transcription was the target, (±)-trans-3-flavanol-3-benzoate, lacking all the hydroxyl groups, was the most effective both in lowering MMP-9 promoter activity and consequently protein secretion, and in inhibiting nuclear-factor-κB-driven transcription. Our results suggest that the structural requirements for enzyme inhibition are different from those necessary for targeting gene expression.
IT 1486-48-2P 1486-51-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of gallocatechin-3-gallate analogs; structure-activity study for the inhibition of matrix metalloproteinase-9 activity and gene expression by analogs of gallocatechin-3-gallate)
RN 1486-48-2 CAPLUS
CN Benzoic acid, 3,4,5-tris(phenylmethoxy)- (CA INDEX NAME)



RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 19 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:1103728 CAPLUS
DN 143:386777
TI Process for the preparation of carboxylic acid compound
IN Hibino, Hiroaki; Yoshida, Tomoyasu
PA Sumitomo Chemical Company, Limited, Japan
SO PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005095319	A1	20051013	WO 2005-JP6578	20050329
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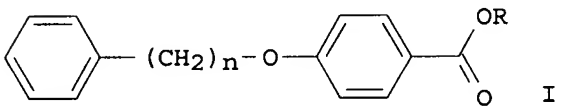
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1739071	A1	20070103	EP 2005-721717	20050329
	R: CH, DE, FR, GB, IT, LI				
	CN 1938253	A	20070328	CN 2005-80009755	20050329
	JP 2005314406	A	20051110	JP 2005-101691	20050331
	US 2007197824	A1	20070823	US 2006-594501	20060928
PRAI	JP 2004-108760	A	20040401		
	WO 2005-JP6578	W	20050329		

OS CASREACT 143:386777; MARPAT 143:386777
GI



I

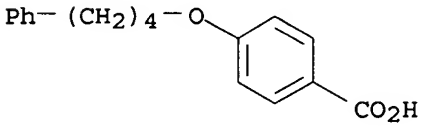
AB A process for the preparation of title compds. of formula I [n = 1-6, R = H] comprising hydrolysis of mixture of a compound of formula I (R = alkyl, n is defined as above) and 4-ROC6H4CO2R (R is defined as above) at PH 4~8 is disclosed. For example, substitution of Me 4-hydroxybenzoate with 4-phenyl-1-chlorobutane gave Me 4-(4-phenylbutoxy)benzoate in 96% yield with the byproduct of Me 4-methoxybenzoate. Hydrolysis of this ester mixture by adjustment of PH 4~8, selectively provided 4-(4-

phenylbutoxy)benzoic acid in 99.6% yield.

IT 30131-16-9P, 4-(4-Phenylbutoxy)benzoic acid
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(selectively preparation of carboxylic acids by hydrolysis of carboxylate esters)

RN 30131-16-9 CAPLUS

CN Benzoic acid, 4-(4-phenylbutoxy)- (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 20 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:962196 CAPLUS

DN 143:266597

TI Preparation of benzamides and nitrogen-heterocycle carboxamides as NMDA NR2B receptor antagonists with therapeutic uses

IN Kawai, Makoto; Kawamura, Mitsuhiro; Sakurada, Isao; Morita, Asato

PA Pfizer Japan, Inc., Japan; Pfizer Inc.

SO PCT Int. Appl., 213 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005080317	A2	20050901	WO 2005-IB258	20050201
	WO 2005080317	A3	20060216		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2555970	A1	20050901	CA 2005-2555970	20050201
	EP 1716100	A2	20061102	EP 2005-702407	20050201
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
	BR 2005007636	A	20070710	BR 2005-7636	20050201
	US 2007167452	A1	20070719	US 2006-597868	20060810
	MX 2006PA09198	A	20061003	MX 2006-PA9198	20060811
PRAI	US 2004-544258P	P	20040211		
	WO 2005-IB258	W	20050201		

OS MARPAT 143:266597

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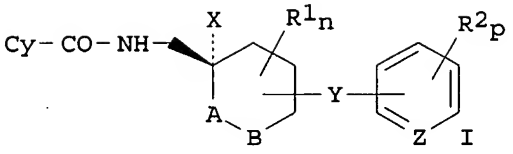
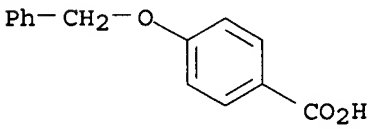


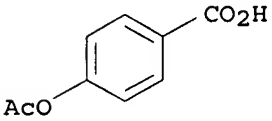
AB The present invention relates to benzamides and nitrogen-heterocycle carboxamides (shown as I; variables defined below; e.g. 4-hydroxy-N-[[cis-4-(phenoxymethyl)cyclohexyl]methyl]benzamide) or a pharmaceutically acceptable salt or solvate thereof, to processes for the preparation of, intermediates used in the preparation of, compns. containing such compds. and the uses of such compds. as antagonists of the NMDA NR2B receptor. For I: A and B = CH2 or O, with the proviso that A and B are not simultaneously O; Cy = one of 30 ring radicals, e.g. 4-hydroxyphenyl and 1H-pyrazol-4-yl (un)substituted by 1-3 hydroxy, halogen, C1-6alkyl, C1-6alkoxy, C1-6 haloalkyl, C1-6alkylamino and amino; R1 and R2 = hydroxy, halogen, C1-6alkyl, C1-6alkoxy, C1-6 haloalkyl and C3-8 cycloalkyl; n = 0-4; X is H, hydroxy, halogen or C1-6alkoxy; Y is oxy, thio, a 1-4 membered alkylene, a 2-4 membered alkylene ether, 2-4 membered alkylene thioether or an oxyethyleneoxy group, (un)substituted by 1-4 hydroxy, halogen, C1-6alkyl, C1-6alkoxy and C1-6 haloalkyl; Z is CH or N; and p = 0-5 when Z is CH or 0-4 when Z is N; when p = ≥2, two of R2s may be taken together with the C atoms to which they are attached to form a 5-8 membered cycloalkyl ring. Although the methods of preparation are not claimed, >130 example prepns. for I and >180 for intermediates are included. For example, II was prepared by condensation of 4-(benzyloxy)-N-[[cis-4-(hydroxymethyl)cyclohexyl]methyl]benzamide with phenol using DIAD and PPh3 followed by debenzylation via hydrogenation over 10 % Pd-C. Results for some I in NR2B and human dofetilide binding assays are tabulated.

IT 1486-51-7, 4-(Benzyloxy)benzoic acid 2345-34-8, 4-Acetoxybenzoic acid 25458-44-0, 4-(Methoxymethoxy)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzamides and nitrogen-heterocycle carboxamides as NMDA NR2B receptor antagonists with therapeutic uses)

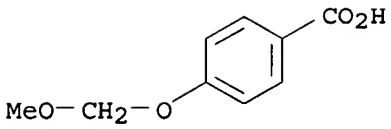
RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



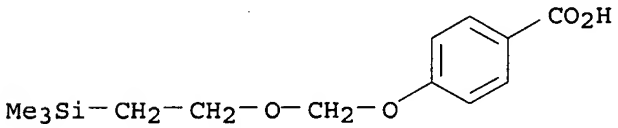
RN 2345-34-8 CAPLUS
CN Benzoic acid, 4-(acetyloxy)- (CA INDEX NAME)



RN 25458-44-0 CAPLUS
CN Benzoic acid, 4-(methoxymethoxy)- (CA INDEX NAME)



IT 863565-41-7P, 4-[[2-(Trimethylsilyl)ethoxy]methoxy]benzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzamides and nitrogen-heterocycle carboxamides as NMDA NR2B receptor antagonists with therapeutic uses)
RN 863565-41-7 CAPLUS
CN Benzoic acid, 4-[[2-(trimethylsilyl)ethoxy]methoxy]- (9CI) (CA INDEX NAME)



L15 ANSWER 21 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:588911 CAPLUS
DN 143:115353
TI Benzamide derivatives bearing a cyclopropylaminoacarbonyl substituent useful as cytokine inhibitors
IN Brown, Dearg Sutherland; Cumming, John Graham; Nash, Ian Alun
PA Astrazeneca AB, Swed.; Astrazeneca UK Limited
SO PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005061465	A1	20050707	WO 2004-GB5241	20041215
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004303579	A1	20050707	AU 2004-303579	20041215
	CA 2547617	A1	20050707	CA 2004-2547617	20041215
	EP 1699766	A1	20060913	EP 2004-806056	20041215
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	CN 1918134	A	20070221	CN 2004-80041887	20041215
	BR 2004017844	A	20070417	BR 2004-17844	20041215
	JP 2007516979	T	20070628	JP 2006-544544	20041215
	MX 2006PA06660	A	20060811	MX 2006-PA6660	20060612
	IN 2006DN03812	A	20070713	IN 2006-DN3812	20060703
	NO 2006003330	A	20060914	NO 2006-3330	20060718
	US 2007135440	A1	20070614	US 2006-581305	20061012

PRAI GB 2003-29572 A 20031220
WO 2004-GB5241 W 20041215
OS MARPAT 143:115353
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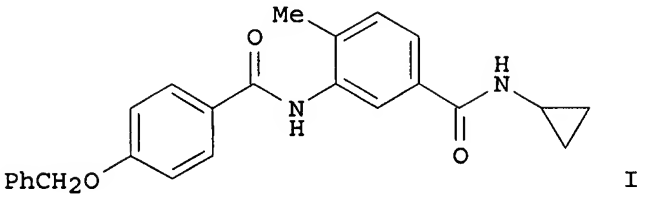
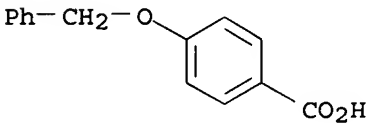


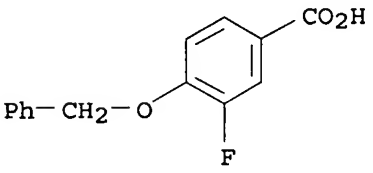
I

AB The invention concerns a the title compds., or pharmaceutically-acceptable salts; processes for their preparation, pharmaceutical compns. containing them and their use in the treatment of diseases or medical conditions mediated by cytokines. E.g., I was prepared from 4-benzyloxybenzoic acid and 3-amino-N-cyclopropyl-4-methylbenzamide. Biol. assays include p38 kinase inhibitory, TNF-inhibitory and antiarthritic effects of the compds.

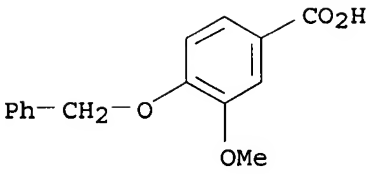
IT 1486-51-7, 4-Benzyloxybenzoic acid 152552-64-2, 4-Benzyloxy-3-fluorobenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzamide derivs. bearing a cyclopropylaminoacarbonyl substituent useful as cytokine inhibitors)
RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



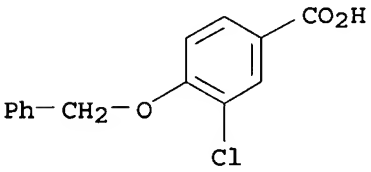
RN 152552-64-2 CAPLUS
CN Benzoic acid, 3-fluoro-4-(phenylmethoxy)- (CA INDEX NAME)



IT 1486-53-9P, 4-Benzyloxy-3-methoxybenzoic acid 106931-79-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(benzamide derivs. bearing a cyclopropylaminoacarbonyl substituent useful as cytokine inhibitors)
RN 1486-53-9 CAPLUS
CN Benzoic acid, 3-methoxy-4-(phenylmethoxy)- (CA INDEX NAME)

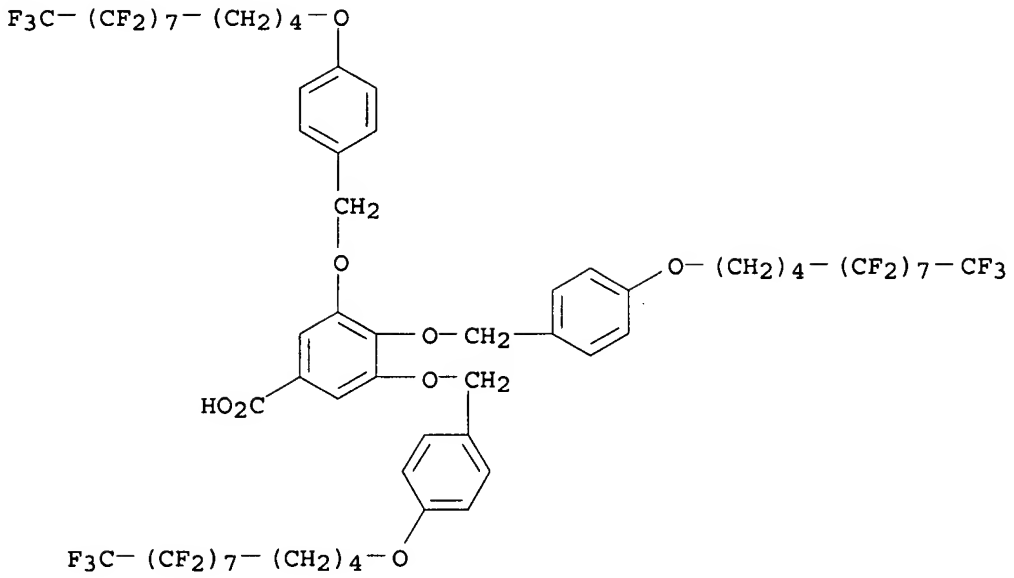


RN 106931-79-7 CAPLUS
CN Benzoic acid, 3-chloro-4-(phenylmethoxy)- (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 22 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:406722 CAPLUS
DN 143:121084
TI Alignment of Perfluorinated Supramolecular Columns on the Surfaces of Various Self-Assembled Monolayers
AU Lee, Eun Ho; Yoon, Dong Ki; Jung, Jin Mi; Lee, Su Rim; Kim, Yun Ho; Kim, Yeon-A.; Kim, Guncheol; Jung, Hee-Tae
CS Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology, Daejeon, 305-701, S. Korea
SO Macromolecules (2005), 38(12), 5152-5157
CODEN: MAMOBX; ISSN: 0024-9297
PB American Chemical Society
DT Journal
LA English
AB We studied the orientation of the hexagonal columnar mesophase formed by self-organization of a perfluorinated supramol. dendrimer containing a carboxyl (-COOH) headgroup and three perfluorinated (-CF3) tails at surfaces modified with self-assembled monolayers (SAMs). The SAM-modified surfaces studied were composed of an Au(111) substrate modified with one of five types of SAM. The SAM mols. used all had an -SH headgroup, but different terminal groups (-CF3, -CH3, and -OH) and different spacer chain lengths. Atomic force microscopy (AFM), transmission electron microscopy (TEM), and contact angle microscopy results revealed that the lattice parameters and structure of the perfluorinated supramol. dendrimer are retained, but the orientation of the columns is strongly affected by the characteristics of the SAM surface. The supramol. columns took on a planar alignment on the -CF3 and -OH terminated SAM surfaces, but exhibited a perpendicular orientation on the -CH3 terminated SAM surface. These variations in column alignment can be attributed to the types of mol. interactions between the terminal groups of the SAM mols. and the perfluorinated core/tails of the supramol. columns. However, the surface morphol. and orientation was not affected by changing the space chain length of the SAM mols. used.
IT 183578-50-9
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(perfluorinated supramol.; alignment of perfluorinated supramol. self-aggregate on SAM)
RN 183578-50-9 CAPLUS
CN Benzoic acid, 3,4,5-tris[[4-[(5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heptadecafluorododecyl)oxy]phenyl]methoxy]- (CA INDEX NAME)

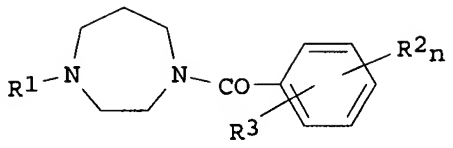


RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 23 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:395292 CAPLUS
DN 142:430314
TI Preparation of (1H-1,4-diazepan-1-yl)(phenyl)methanones as histamine H3 functional antagonists for treating neurological disorders
IN Bruton, Gordon; Huxley, Anthony; Orlek, Barry Sidney; Rana, Kishore Kalidas
PA Glaxo Group Limited, UK
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005040144	A1	20050506	WO 2004-EP11619	20041014
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1675838	A1	20060705	EP 2004-765973	20041014
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR				
	JP 2007508346	T	20070405	JP 2006-534702	20041014
PRAI	GB 2003-24159	A	20031015		
	WO 2004-EP11619	W	20041014		

OS CASREACT 142:430314; MARPAT 142:430314
GI



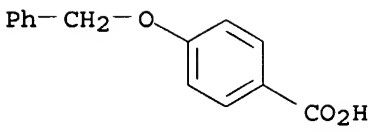
I

AB The present invention relates to novel diazepanyl derivs. (shown as I; variables defined below; e.g. 4'-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]-4-biphenylcarbonitrile (II)) having pharmacol. activity, processes for their preparation, to compns. containing them and to their use in the treatment of neurol. disorders. For I: R1 = branched C3-6 alkyl, C3-5 cycloalkyl or C1-4 alkylC3-4 cycloalkyl; R2 = halo, C1-6 alkyl, C1-6 alkoxy, cyano, amino or trifluoromethyl; n = 0-2; R3 = X-aryl, X-heteroaryl, X-heterocyclyl, X-arylaryl, X-arylheteroaryl, X-arylheterocyclyl, X-heteroarylaryl, X-heteroarylheteroaryl, X-heteroarylheterocyclyl, X-heterocyclylaryl, X-heterocyclylheteroaryl or X-heterocyclylheterocyclyl; such that when R3 = X-piperidinyl, X-piperidinylaryl, X-piperidinylheteroaryl or X-piperidinylheterocyclyl said piperidinyl group is attached to X via a N atom; wherein R3 is attached to the Ph group of I at the 3 or 4 position; X = a bond, O, CO, SO2, CH2O, OCH2, NR4, NR4CO or C1-6-alkyl. R4 = H or C1-6 alkyl; wherein said aryl, heteroaryl or heterocyclyl groups of R3 may be (un)substituted by ≥1 (e.g. 1, 2 or 3) halo, hydroxy, cyano, nitro, oxo, haloC1-6 alkyl, haloC1-6 alkoxy, C1-6 alkyl, C1-6 alkoxy, arylC1-6 alkoxy, C1-6 alkylthio, C1-6 alkoxyC1-6 alkyl, C3-7 cycloalkylC1-6 alkoxy, C3-7 cycloalkylcarbonyl, -COC1-6 alkyl, C1-6 alkoxycarbonyl, arylC1-6 alkyl, heteroarylC1-6-alkyl, heterocyclylC1-6 alkyl, C1-6 alkylsulfonyl, C1-6 alkylsulfinyl, C1-6 alkylsulfonyloxy, C1-6 alkylsulfonylC1-6 alkyl, arylsulfonyl, arylsulfonyloxy, arylsulfonylC1-6 alkyl, aryloxy, CO-aryl, CO-heterocyclyl, CO-heteroaryl, C1-6 alkylsulfonamidoC1-6 alkyl, C1-6 alkylamidoC1-6 alkyl, arylsulfonamido, arylaminosulfonyl, arylsulfonamidoC1-6 alkyl, arylcarboxamidoC1-6 alkyl, aroylC1-6 alkyl, arylC1-6 alkanoyl, NR15R16, NR15CO-aryl, NR15CO-heterocyclyl, NR15CO-heteroaryl, CONR15R16, NR15COR16, NR15SO2R16 or SO2NR15R16 groups, wherein R15 and R16 = independently H or C1-6 alkyl. Although the methods of preparation are not claimed, 58 example prepns. and/or characterization data sets for I are included; example prepns. for intermediates are also included. For example, II was prepared from 1-(cyclobutyl)hexahydro-1H-1,4-diazepine dihydrochloride and 4'-cyano-4-biphenylcarboxylic acid using diethylaminomethylpolystyrene, HOBT and EDC in CH2Cl2. The diazepine reactant was prepared in 2 steps starting from tert-Bu hexahydro-1H-1,4-diazepine-1-carboxylate and cyclobutanone followed by deprotection at N. The 58 example I were tested in the histamine H3 functional antagonist assay and exhibited pKb values > 8.0. Most particularly, the hydrochlorides of II, 1-[4'-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]biphenyl-4-yl]ethanone, 1-cyclobutyl-4-[[4-[6-(trifluoromethyl)-3-pyridinyl]phenyl]carbonyl]hexahydro-1H-1,4-diazepine, 6-[4-[(4-cyclobutylhexahydro-1H-1,4-diazepin-1-yl)carbonyl]phenyl]-3-cyanopyridine and 1-Cyclobutyl-4-[[4-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl]carbonyl]hexahydro-1H-1,4-diazepine exhibited pKb values >9.5. Most of the 58 example I were tested in the histamine H1 functional antagonist assay and exhibited antagonism < 7.0 pKb; most of these exhibited antagonism < 6.0 pKb.

IT 1486-51-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (1H-1,4-diazepan-1-yl)(phenyl)methanones as histamine H3 functional antagonists for treating neurol. disorders)

RN 1486-51-7 CAPLUS

CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 24 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:324138 CAPLUS
DN 142:392428
TI Preparation of heterocyclic compounds as antifungal agents
IN Nakamoto, Kazutaka; Tsukada, Itaru; Tanaka, Keigo; Matsukura, Masayuki; Haneda, Toru; Inoue, Satoshi; Ueda, Norihiro; Abe, Shinya; Hata, Katsura; Watanabe, Naoaki
PA Eisai Co., Ltd., Japan
SO PCT Int. Appl., 418 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005033079	A1	20050414	WO 2004-JP14063	20040927
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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	EP 1669348	A1	20060614	EP 2004-788159	20040927
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	WO 2006016548	A1	20060216	WO 2005-JP14505	20050808
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	EP 1782811	A1	20070509	EP 2005-768893	20050808
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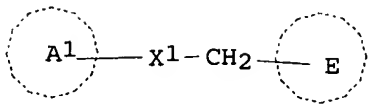
	US 2007105943	A1	20070510	US 2006-573890	20060329
PRAI	JP 2003-342273	A	20030930		
	JP 2004-68186	A	20040310		
	JP 2004-232617	A	20040809		
	WO 2004-JP14063	W	20040927		
	JP 2005-82760	A	20050322		
	WO 2005-JP14505	W	20050808		

OS MARPAT 142:392428
GI



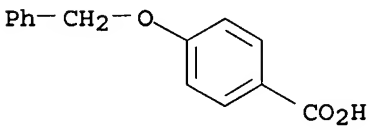
I

AB The title compds., e.g. I [ring A1 is optionally substituted 3-pyridyl, optionally substituted quinolyl, etc.; X1 is NHCO, etc.; and ring E is furyl, thienyl, pyrrolyl, Ph, pyridyl, tetrazolyl, thiazolyl, or pyrazolyl; provided that A1 may have one to three substituents and E has one or two substituents], are prepared 2,6-Diamino-N-(5-(4-fluorophenoxy)furan-2-ylmethyl)nicotinamide was prepared in a multistep process. Compds. of this invention in vitro showed MIC values of 0.1 μg/mL to 6.25 μg/mL against Candida.

IT 1486-51-7, 4-Benzyloxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heterocyclic compds. as antifungal agents)

RN 1486-51-7 CAPLUS

CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 25 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:1127319 CAPLUS
DN 142:74357
TI Preparation of new benzamides for use in pharmaceutical compositions as peroxisome proliferator-activated receptor γ (PPARγ) modulators
IN Ferdandez Serrat, Anna; Serra Comas, Carme; Balsa Lopez, Dolors; Llebaria Soldevila, Amadeu; Farrerons Gallemi, Carles; Miquel Bono, Ignacio Jose; Catena Ruiz, Juan Lorenzo; Lagunas Arnal, Carmen; Cordomi Montoya, Arnau; Salcedo Roca, Carolina; Toledo Mesa, Natividad; Marrero Gonzalez, Pedro; Haro Bautista, Diego; Fernandez Garcia, Andres
PA Laboratorios S.A.L.V.A.T., S.A., Spain
SO PCT Int. Appl., 113 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004110983	A2	20041223	WO 2004-EP6330	20040611

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,

SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

	AU 2004247389	A1	20041223	AU 2004-247389	20040611
	CA 2528231	A1	20041223	CA 2004-2528231	20040611
	EP 1644321	A2	20060412	EP 2004-739820	20040611
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	BR 2004011412	A	20060725	BR 2004-11412	20040611
	CN 1835914	A	20060920	CN 2004-80023119	20040611
	JP 2006527233	T	20061130	JP 2006-515904	20040611
	MX 2005PA13653	A	20060224	MX 2005-PA13653	20051213
	US 2006160894	A1	20060720	US 2005-560533	20051213
	IN 2006CN00121	A	20070629	IN 2006-CN121	20060110
PRAI	ES 2003-1461	A	20030613		
	WO 2004-EP6330	W	20040611		

OS MARPAT 142:74357

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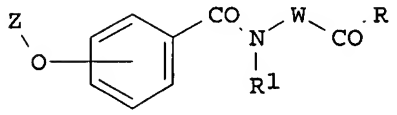


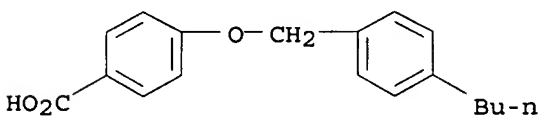
I

AB Benzamides, such as I [R = OH, NH2, alkoxy, alkylamino, etc.; R1 = H, alkyl, benzyl, etc.; W = alkylene, aryl substituted alkylene; Z = benzyl, biphenylmethyl, phenylalkyl, etc.], were prepared for use in the prophylactic and/or curative treatment of a condition or a disease mediated by the PPARγ. These benzamides are claimed for use in the treatment of metabolic diseases, such as non-insulin-dependent diabetes mellitus, obesity, hypercholesterolemia and other lipid-mediated pathologies, as well as for treatment of cardiovascular disease associated with metabolic syndrome, treatment of inflammation or an inflammatory processes, such as rheumatoid arthritis, atherosclerosis, psoriasis and intestinal inflammatory disease, for treatment of cancer, skin wound healing or cutaneous disorders associated with an anomalous differentiation of epidermic cells, and for treatment of bone disease, particularly osteoporosis. Thus, the L-phenylalanine derivative, (S)-PhCH2O-4-C6H4CH2CH(CO2Me)NHCOC6H4-4-OCH2C6H4-4-OPh, is an example of the target benzamides prepared The prepared benzamides were assayed for PPARγ binding affinity and were evaluated for their PPARγ agonist/antagonist functional activity.

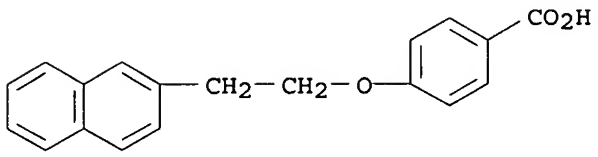
IT 158938-04-6P 221265-67-4P 647007-55-4P
814920-61-1P 814920-63-3P 814920-65-5P
814920-74-6P 814920-77-9P 814920-85-9P
814920-86-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of new benzamides for use in pharmaceutical compns. as peroxisome proliferator-activated receptor γ (PPARγ) modulators)

RN 158938-04-6 CAPLUS

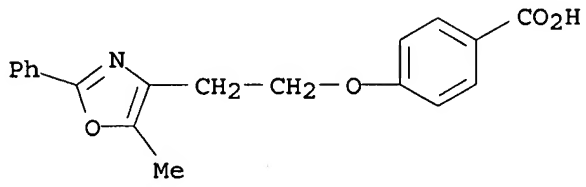
CN Benzoic acid, 4-[(4-butylphenyl)methoxy]- (9CI) (CA INDEX NAME)



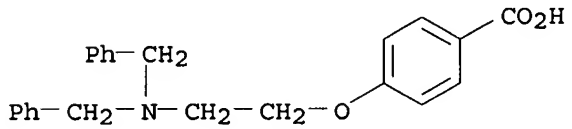
RN 221265-67-4 CAPLUS
CN Benzoic acid, 4-[2-(2-naphthalenyl)ethoxy]- (9CI) (CA INDEX NAME)



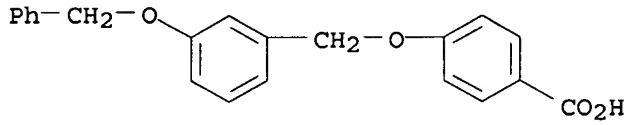
RN 647007-55-4 CAPLUS
CN Benzoic acid, 4-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]- (9CI) (CA INDEX NAME)



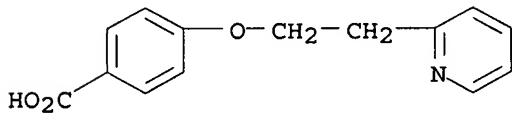
RN 814920-61-1 CAPLUS
CN Benzoic acid, 4-[2-[bis(phenylmethyl)amino]ethoxy]- (9CI) (CA INDEX NAME)



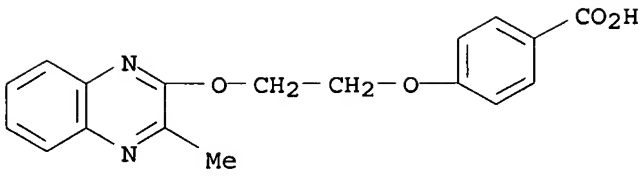
RN 814920-63-3 CAPLUS
CN Benzoic acid, 4-[[3-(phenylmethoxy)phenyl]methoxy]- (9CI) (CA INDEX NAME)



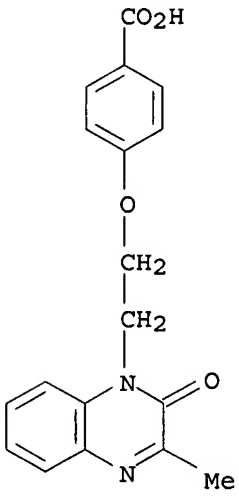
RN 814920-65-5 CAPLUS
CN Benzoic acid, 4-[2-(2-pyridinyl)ethoxy]- (9CI) (CA INDEX NAME)



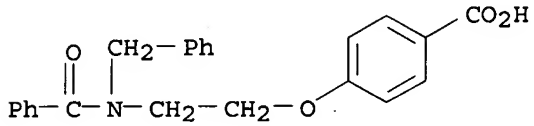
RN 814920-74-6 CAPLUS
CN Benzoic acid, 4-[2-[(3-methyl-2-quinoxalinyl)oxy]ethoxy]- (9CI) (CA INDEX NAME)



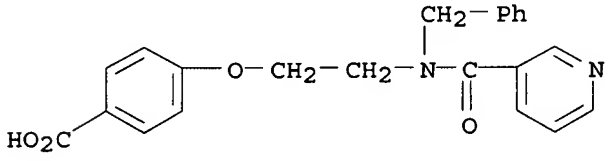
RN 814920-77-9 CAPLUS
CN Benzoic acid, 4-[2-(3-methyl-2-oxo-1(2H)-quinoxalinyl)ethoxy]- (9CI) (CA INDEX NAME)



RN 814920-85-9 CAPLUS
CN Benzoic acid, 4-[2-[benzoyl(phenylmethyl)amino]ethoxy]- (9CI) (CA INDEX NAME)

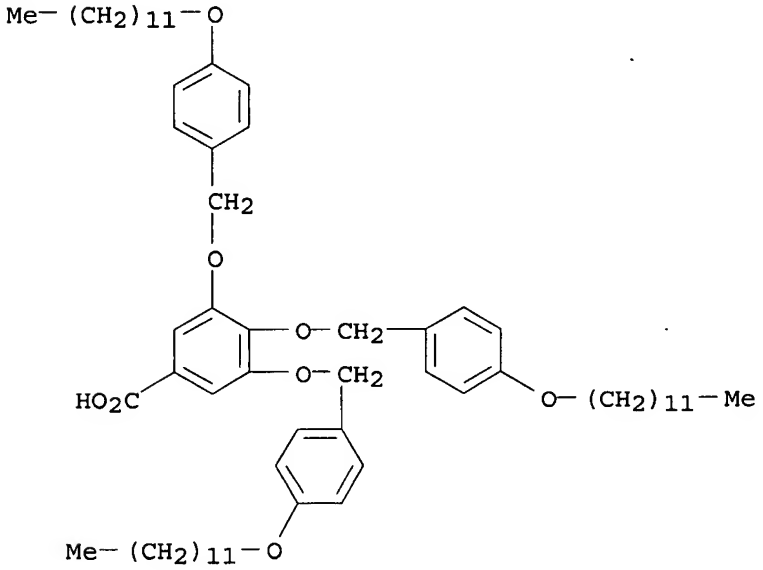


RN 814920-86-0 CAPLUS
CN Benzoic acid, 4-[2-[(phenylmethyl)(3-pyridinylcarbonyl)amino]ethoxy]- (9CI) (CA INDEX NAME)



L15 ANSWER 26 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:595225 CAPLUS
DN 141:302104
TI Expression of Molecular Chirality and Two-Dimensional Supramolecular Self-Assembly of Chiral, Racemic, and Achiral Monodendrons at the Liquid-Solid Interface

AU Mamdouh, Wael; Ujii, Hiroshi; Dulcey, Andres E.; Percec, Virgil; De Feyter, Steven; De Schryver, Frans C.
CS Department of Chemistry, Laboratory of Photochemistry and Spectroscopy, Katholieke Universiteit Leuven, Louvain, 3001, Belg.
SO Langmuir (2004), 20(18), 7678-7685
CODEN: LANGD5; ISSN: 0743-7463
PB American Chemical Society
DT Journal
LA English
AB We have investigated the two-dimensional ordering of chiral and achiral monodendrons at the liquid-solid interface. The chiral mols. self-assemble into extended arrays of dimers. As expected, the R enantiomer forms the mirror image type pattern of the chiral two-dimensional structure formed by the S enantiomer. A racemic mixture applied from solution onto the substrate undergoes spontaneous segregation: the enantiomers sep. on the surface and appear in different domains. In contrast to the chiral mols., the achiral analog self-assembles into cyclic tetramers. Moreover, the pattern formed by the achiral mol. strongly depends on the solvent used. In the case of 1-phenyloctane, solvent mols. are coadsorbed in a 2:1 (dendron:solvent) ratio whereas in 1-octanol, no solvent mols. are coadsorbed. By the appropriate solvent choice, the distance between the potential "supramol. containers" can be influenced.
IT 110934-58-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; to synthesize chiral, racemic, and achiral monodendrons)
RN 110934-58-2 CAPLUS
CN Benzoic acid, 3,4,5-tris[[4-(dodecyloxy)phenyl]methoxy]- (CA INDEX NAME)



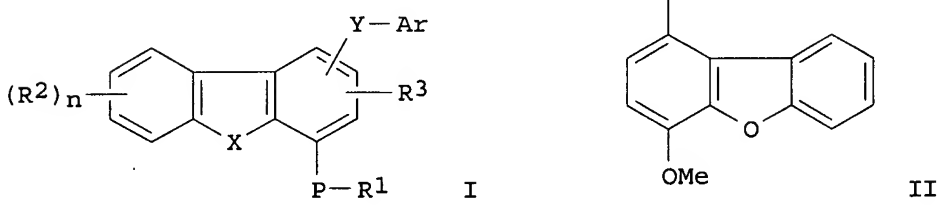
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 27 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:370918 CAPLUS
DN 140:391192
TI Preparation of dibenzofuran/dibenzothiophene derivatives useful for the treatment of inflammatory and allergic disorders
IN Balasubramanian, Gopalan; Gharat, Laxmikant Atmaram; Lakdawala, Aftab Dawoodbhai; Anupindi, Raghu Ram
PA Glenmark Pharmaceuticals Ltd., India
SO PCT Int. Appl., 254 pp.
CODEN: PIXXD2

DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004037805	A1	20040506	WO 2003-IB4442	20031008
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	IN 2002MU00922	A	20050304	IN 2002-MU922	20021023
	CA 2503015	A1	20040506	CA 2003-2503015	20031008
	AU 2003269317	A1	20040513	AU 2003-269317	20031008
	EP 1554262	A1	20050720	EP 2003-751096	20031008
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	BR 2003014721	A	20050802	BR 2003-14721	20031008
	CN 1729181	A	20060201	CN 2003-80107246	20031008
	JP 2006506379	T	20060223	JP 2004-546246	20031008
	ZA 2005002969	A	20060222	ZA 2005-2969	20050413
	US 2006178418	A1	20060810	US 2005-532273	20050926
	US 7238725	B2	20070703		
PRAI	IN 2002-MU922	A	20021023		
	WO 2003-IB4442	W	20031008		

OS MARPAT 140:391192
GI

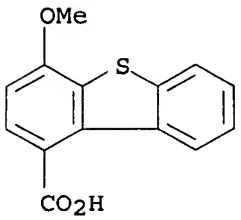


AB Title compds. I [R1-3 = H, alk(en/yn)yl, cycloalkyl, etc.; P = O, S; n = 0-4; Ar = (un)substituted aryl, etc.; Y = carboxamido, aminosulfonyl, etc.] are prepared For instance, 4-methoxydibenzofuran-1-carboxylic acid (preparation given) is converted to the corresponding acid chloride (PhH, SOCl2, reflux, 4 h) and treated with 4-amino-3,5-dichloropyridine (DMF/THF, NaH, -10°) to give II. II has IC50 = 0.8 nM for PDE4. I are useful for the treatment of inflammatory conditions, diseases of the central nervous and insulin resistant diabetes.

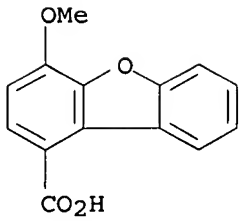
IT 58108-18-2P 667941-07-3P, 4-Methoxydibenzofuran-1-carboxylic acid 685873-43-2P, 3-(2-Nitrophenoxy)-4-methoxybenzoic acid 685873-44-3P, 3-(2-Aminophenoxy)-4-methoxybenzoic acid 685873-46-5P 685873-48-7P, 3-(2-Nitro-4-trifluoromethylphenoxy)-4-methoxybenzoic acid

685873-49-8P, 3-(2-Amino-4-trifluoromethylphenoxy)-4-methoxybenzoic acid 685873-50-1P, 4-Methoxy-8-trifluoromethyldibenzofuran-1-carboxylic acid 685873-52-3P, 3-(2-Nitro-4-trifluoromethylphenoxy)-4-difluoromethoxybenzoic acid 685873-53-4P, 3-(2-Amino-4-trifluoromethylphenoxy)-4-difluoromethoxybenzoic acid 685873-54-5P, 4-Difluoromethoxy-8-trifluoromethyldibenzofuran-1-carboxylic acid 685873-56-7P 685873-58-9P, 3-(2-Nitrophenoxy)-4-difluoromethoxybenzoic acid 685873-59-0P, 3-(2-Aminophenoxy)-4-difluoromethoxybenzoic acid 685873-60-3P, 4-Difluoromethoxydibenzofuran-1-carboxylic acid 685873-62-5P 685873-67-0P, 4-Cyclopropylmethoxydibenzofuran-1-carboxylic acid 685873-69-2P, 4-Isopropyloxydibenzofuran-1-carboxylic acid 685873-71-6P, 4-Benzyloxydibenzofuran-1-carboxylic acid 685873-74-9P, 4-Methoxy-8-nitrodibenzofuran-1-carboxylic acid 685873-75-0P, 4-Methoxy-8-aminodibenzofuran-1-carboxylic acid 685873-76-1P, 4-Methoxy-8-chlorodibenzofuran-1-carboxylic acid 685873-77-2P, 4-Methoxy-8-bromodibenzofuran-1-carboxylic acid 685873-78-3P, 4-Methoxy-8-iododibenzofuran-1-carboxylic acid 685873-94-3P, 4-Difluoromethoxy-8-nitrodibenzofuran-1-carboxylic acid 685874-00-4P, 4-Ethoxydibenzofuran-1-carboxylic acid 685874-11-7P, 1-Methoxy-9H-4-carbazolecarboxylic acid 685874-24-2P, 6-Chloro-9-(4-fluorobenzyl)-1-methoxy-9H-4-carbazolecarboxylic acid 685874-30-0P, 4-Ethoxydibenzothiophene-1-carboxylic acid 685874-34-4P, 4-Benzyloxydibenzothiophene-1-carboxylic acid 685874-38-8P, 6-Ethyl-4-methoxydibenzothiophene-1-carboxylic acid 685874-41-3P, 4-Difluoromethoxydibenzothiophen e-1-carboxylic acid 685875-01-8P, 4-Methoxy-8-cyanodibenzofuran-1-carboxylic acid 685875-27-8P, 6-Chloro-1-methoxy-9H-4-carbazolecarboxylic acid 685875-43-8P 685875-46-1P, 9-Benzyl-1-methoxy-9H-4-carbazolecarboxylic acid 685875-50-7P, 9-Benzyl-1-ethoxy-9H-4-carbazolecarboxylic acid 685875-54-1P, 9-Benzyl-6-chloro-1-ethoxy-9H-4-carbazolecarboxylic acid 685875-61-0P, 8-Chloro-9-cyclohexylmethyl-1-methoxy-9H-4-carbazolecarboxylic acid 685875-65-4P, 8-Chloro-9-(4-Fluorobenzyl)-1-methoxy-9H-4-carbazolecarboxylic acid 685875-69-8P , 6-Chloro-1-methoxy-9-methyl-9H-4-carbazolecarboxylic acid 685875-76-7P, 1-Methoxy-9-methyl-9H-4-carbazolecarboxylic acid 685875-88-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dibenzofuran/dibenzothiophene derivs. useful for treatment of inflammatory and allergic disorders)

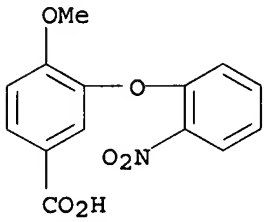
RN 58108-18-2 CAPLUS
CN 1-Dibenzothiophenecarboxylic acid, 4-methoxy- (9CI) (CA INDEX NAME)



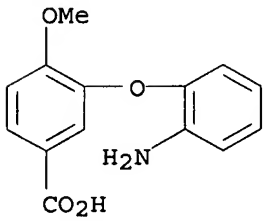
RN 667941-07-3 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 4-methoxy- (5CI, 9CI) (CA INDEX NAME)



RN 685873-43-2 CAPLUS
CN Benzoic acid, 4-methoxy-3-(2-nitrophenoxy)- (9CI) (CA INDEX NAME)



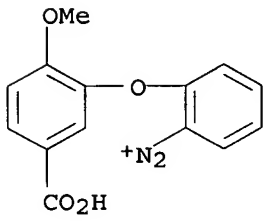
RN 685873-44-3 CAPLUS
CN Benzoic acid, 3-(2-aminophenoxy)-4-methoxy- (9CI) (CA INDEX NAME)



RN 685873-46-5 CAPLUS
CN Benzenediazonium, 2-(5-carboxy-2-methoxyphenoxy)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

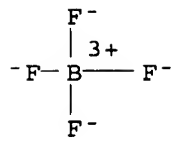
CM 1

CRN 685873-45-4
CMF C14 H11 N2 O4

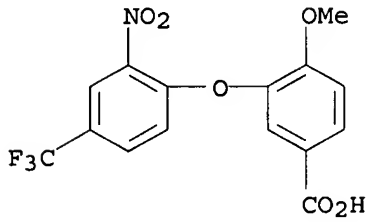


CM 2

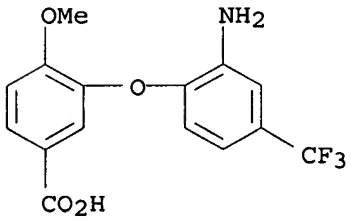
CRN 14874-70-5
CMF B F4
CCI CCS



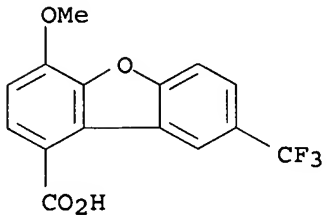
RN 685873-48-7 CAPLUS
CN Benzoic acid, 4-methoxy-3-[2-nitro-4-(trifluoromethyl)phenoxy]- (9CI) (CA INDEX NAME)



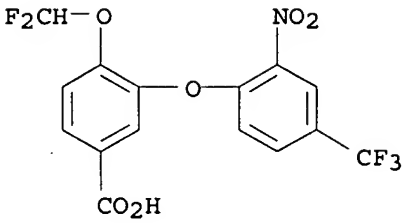
RN 685873-49-8 CAPLUS
CN Benzoic acid, 3-[2-amino-4-(trifluoromethyl)phenoxy]-4-methoxy- (9CI) (CA INDEX NAME)



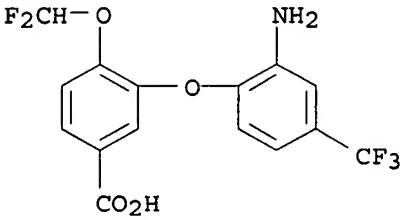
RN 685873-50-1 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 4-methoxy-8-(trifluoromethyl)- (9CI) (CA INDEX NAME)



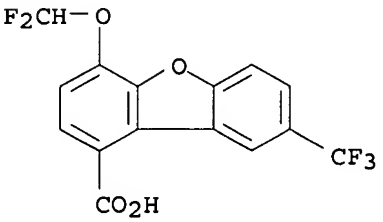
RN 685873-52-3 CAPLUS
CN Benzoic acid, 4-(difluoromethoxy)-3-[2-nitro-4-(trifluoromethyl)phenoxy]- (9CI) (CA INDEX NAME)



RN 685873-53-4 CAPLUS
CN Benzoic acid, 3-[2-amino-4-(trifluoromethyl)phenoxy]-4-(difluoromethoxy)-
(9CI) (CA INDEX NAME)



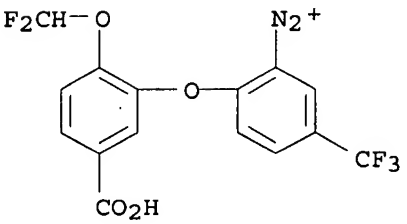
RN 685873-54-5 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 4-(difluoromethoxy)-8-(trifluoromethyl)-
(9CI) (CA INDEX NAME)



RN 685873-56-7 CAPLUS
CN Benzenediazonium, 2-[5-carboxy-2-(difluoromethoxy)phenoxy]-5-
(trifluoromethyl)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

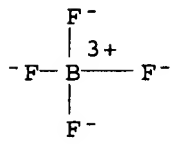
CRN 685873-55-6
CMF C15 H8 F5 N2 O4



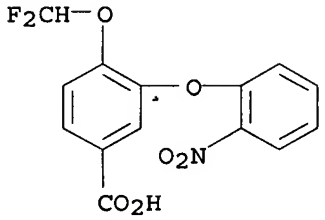
CM 2

CRN 14874-70-5

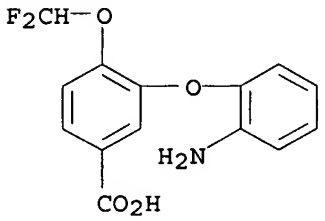
CMF B F4
CCI CCS



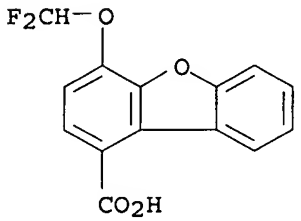
RN 685873-58-9 CAPLUS
CN Benzoic acid, 4-(difluoromethoxy)-3-(2-nitrophenoxy)- (9CI) (CA INDEX NAME)



RN 685873-59-0 CAPLUS
CN Benzoic acid, 3-(2-aminophenoxy)-4-(difluoromethoxy)- (9CI) (CA INDEX NAME)



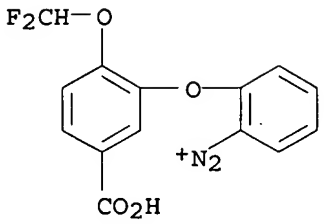
RN 685873-60-3 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 4-(difluoromethoxy)- (9CI) (CA INDEX NAME)



RN 685873-62-5 CAPLUS
CN Benzenediazonium, 2-[5-carboxy-2-(difluoromethoxy)phenoxy]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

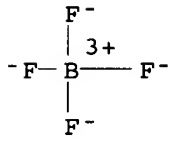
CM 1

CRN 685873-61-4
CMF C14 H9 F2 N2 O4

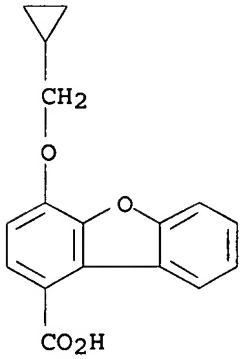


CM 2

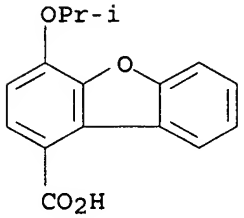
CRN 14874-70-5
CMF B F4
CCI CCS



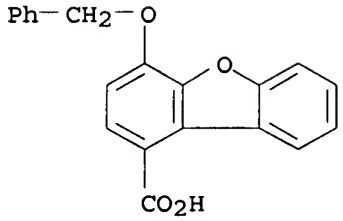
RN 685873-67-0 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 4-(cyclopropylmethoxy)- (9CI) (CA INDEX NAME)



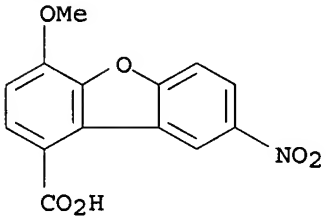
RN 685873-69-2 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 4-(1-methylethoxy)- (9CI) (CA INDEX NAME)



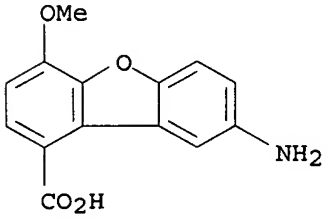
RN 685873-71-6 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



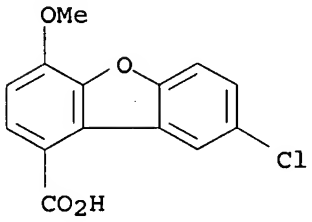
RN 685873-74-9 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 4-methoxy-8-nitro- (9CI) (CA INDEX NAME)



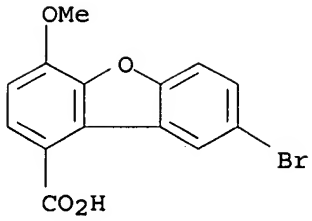
RN 685873-75-0 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 8-amino-4-methoxy- (9CI) (CA INDEX NAME)



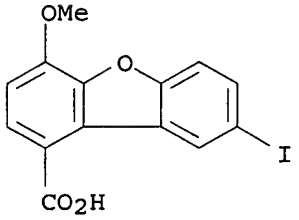
RN 685873-76-1 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 8-chloro-4-methoxy- (9CI) (CA INDEX NAME)



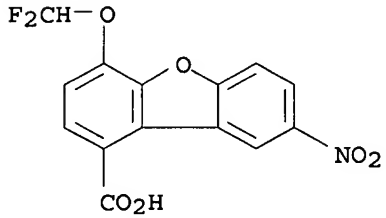
RN 685873-77-2 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 8-bromo-4-methoxy- (9CI) (CA INDEX NAME)



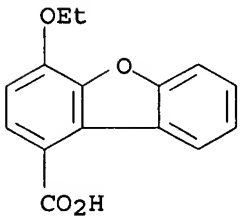
RN 685873-78-3 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 8-iodo-4-methoxy- (9CI) (CA INDEX NAME)



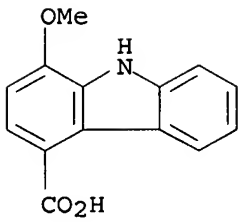
RN 685873-94-3 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 4-(difluoromethoxy)-8-nitro- (9CI) (CA INDEX NAME)



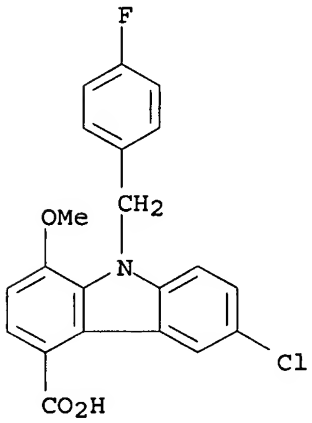
RN 685874-00-4 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 4-ethoxy- (9CI) (CA INDEX NAME)



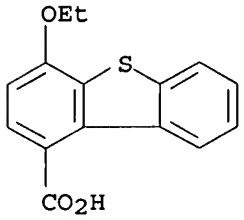
RN 685874-11-7 CAPLUS
CN 9H-Carbazole-4-carboxylic acid, 1-methoxy- (9CI) (CA INDEX NAME)



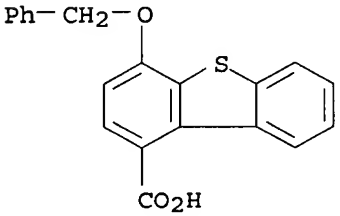
RN 685874-24-2 CAPLUS
CN 9H-Carbazole-4-carboxylic acid, 6-chloro-9-[(4-fluorophenyl)methyl]-1-methoxy- (9CI) (CA INDEX NAME)



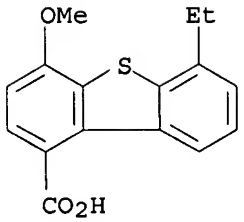
RN 685874-30-0 CAPLUS
CN 1-Dibenzothiophenecarboxylic acid, 4-ethoxy- (9CI) (CA INDEX NAME)



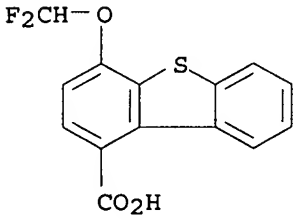
RN 685874-34-4 CAPLUS
CN 1-Dibenzothiophenecarboxylic acid, 4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



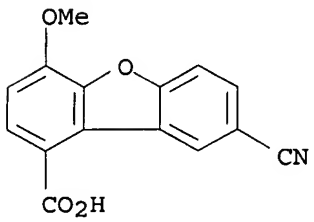
RN 685874-38-8 CAPLUS
CN 1-Dibenzothiophenecarboxylic acid, 6-ethyl-4-methoxy- (9CI) (CA INDEX NAME)



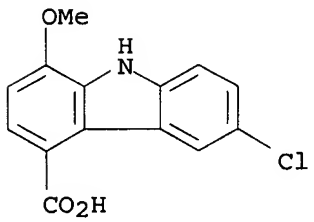
RN 685874-41-3 CAPLUS
CN 1-Dibenzothiophenecarboxylic acid, 4-(difluoromethoxy)- (9CI) (CA INDEX NAME)



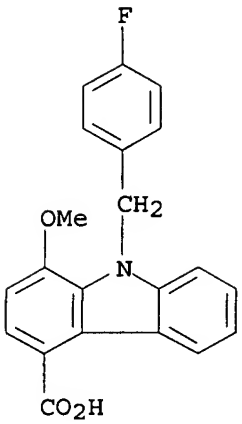
RN 685875-01-8 CAPLUS
CN 1-Dibenzofurancarboxylic acid, 8-cyano-4-methoxy- (9CI) (CA INDEX NAME)



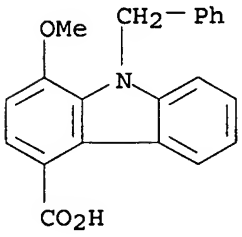
RN 685875-27-8 CAPLUS
CN 9H-Carbazole-4-carboxylic acid, 6-chloro-1-methoxy- (9CI) (CA INDEX NAME)



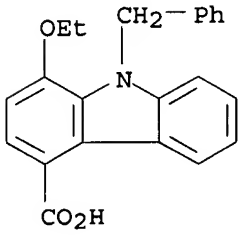
RN 685875-43-8 CAPLUS
CN 9H-Carbazole-4-carboxylic acid, 9-[(4-fluorophenyl)methyl]-1-methoxy- (9CI) (CA INDEX NAME)



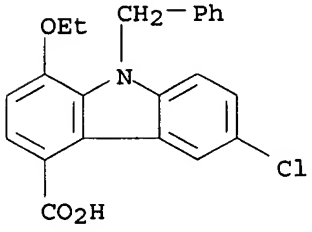
RN 685875-46-1 CAPLUS
CN 9H-Carbazole-4-carboxylic acid, 1-methoxy-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 685875-50-7 CAPLUS
CN 9H-Carbazole-4-carboxylic acid, 1-ethoxy-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

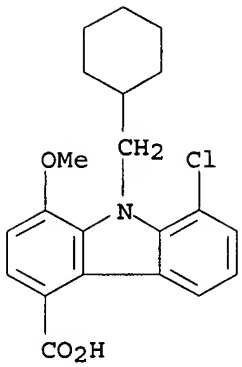


RN 685875-54-1 CAPLUS
CN 9H-Carbazole-4-carboxylic acid, 6-chloro-1-ethoxy-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

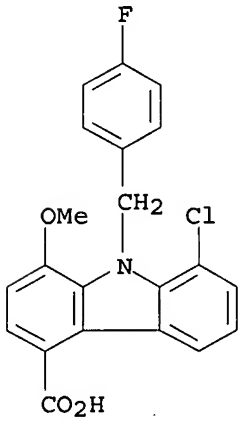


RN 685875-61-0 CAPLUS
CN 9H-Carbazole-4-carboxylic acid, 8-chloro-9-(cyclohexylmethyl)-1-methoxy-

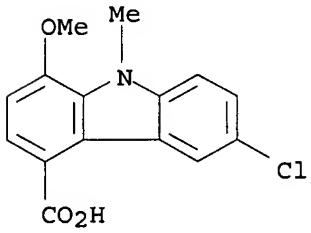
(9CI) (CA INDEX NAME)



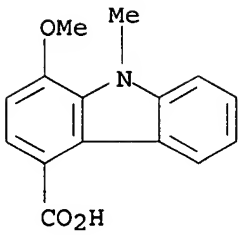
RN 685875-65-4 CAPLUS
CN 9H-Carbazole-4-carboxylic acid, 8-chloro-9-[(4-fluorophenyl)methyl]-1-methoxy- (9CI) (CA INDEX NAME)



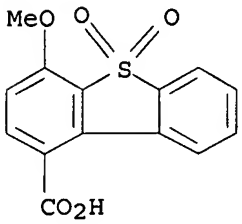
RN 685875-69-8 CAPLUS
CN 9H-Carbazole-4-carboxylic acid, 6-chloro-1-methoxy-9-methyl- (9CI) (CA INDEX NAME)



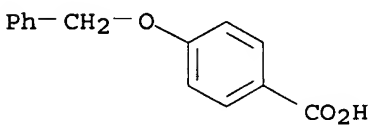
RN 685875-76-7 CAPLUS
CN 9H-Carbazole-4-carboxylic acid, 1-methoxy-9-methyl- (9CI) (CA INDEX NAME)



RN 685875-88-1 CAPLUS
CN 1-Dibenzothiophenecarboxylic acid, 4-methoxy-, 5,5-dioxide (9CI) (CA INDEX NAME)

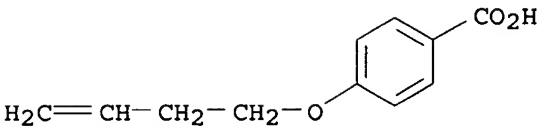


L15 ANSWER 28 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:251181 CAPLUS
DN 140:408008
TI Smectic a elastomers with uniform homeotropic orientation obtained by applying a biaxial mechanical field
AU Nishikawa, Etsushi; Yamamoto, Jun; Yokoyama, Hiroshi; Finkelmann, Heino
CS Yokoyama Nano-Structured Liquid Crystal Project, ERATO, Japan Science and Technology Agency, Tsukuba, 300-2635, Japan
SO Macromolecular Rapid Communications (2004), 25(5), 611-617
CODEN: MRCOE3; ISSN: 1022-1336
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
AB The orientation behavior of a smectic A elastomer is investigated by applying a biaxial mech. field to the elastomer in a swollen state. The network is composed of a siloxane-polymer backbone, a bi-functional cross-linker, and a monomer with a perfluorinated tail. In this work, biaxial deformation is successfully achieved to macroscopically orient the smectic A phase in a uniform, homeotropic fashion. We describe the orientation process in detail and discuss the microstructure of the smectic A phase organized in the monomer, the linear polymer, and the elastomer determined by using X-ray diffraction data.
IT 1486-51-7, p-Benzyloxybenzoic acid 115595-27-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(mesogen synthesis; smectic elastomers with uniform homeotropic orientation by biaxial mech. field)
RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



RN 115595-27-2 CAPLUS

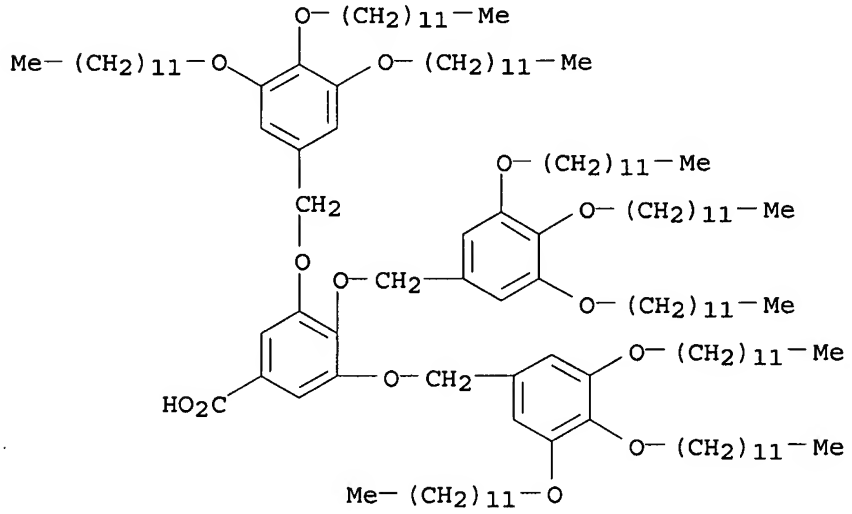
CN Benzoic acid, 4-(3-buten-1-yloxy)- (CA INDEX NAME)



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 29 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:61277 CAPLUS
DN 140:254143
TI Efficiency of Various Lattices from Hard Ball to Soft Ball: Theoretical Study of Thermodynamic Properties of Dendrimer Liquid Crystal from Atomistic Simulation
AU Li, Youyong; Lin, Shiang-Tai; Goddard, William A., III
CS Materials and Process Simulation Center (Mail code 139-74), Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, 91125, USA
SO Journal of the American Chemical Society (2004), 126(6), 1872-1885
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB Self-assembled supramol. organic liquid crystal structures at nanoscale have potential applications in mol. electronics, photonics, and porous nanomaterials. Most of these structures are formed by aggregation of soft spherical supramols., which have soft coronas and overlap each other in the packing process. Our main focus here is to study the possible packing mechanisms via mol. dynamics simulations at the atomistic level. We consider the relative stability of various lattices packed by the soft dendrimer balls, first synthesized and characterized by Percec et al. (J. Am. Chemical Society 1997, 119, 1539) with different packing methods. The dendrons, which form the soft dendrimer balls, have the character of a hard aromatic region from the point of the cone to the edge with C12 alkane "hair". After the dendrons pack into a sphere, the core of the sphere has the hard aromatic groups, while the surface is covered with the C12 alkane "hair". In our studies, we propose three ways to organize the hair on the balls, Smooth/Valentino balls, Sticky/Einstein balls, and Asym./Punk balls, which lead to three different packing mechanisms, Slippery, Sticky, and Anisotropic, resp. We carry out a series of mol. dynamics (MD) studies on three plausible crystal structures (A15, FCC, and BCC) as a function of d. and analyze the MD based on the vibrational d. of state (DoS) method to extract the enthalpy, entropy, and free energies of these systems. We find that anisotropic packed A15 is favored over FCC, BCC lattices. Our predicted X-ray intensities of the best structures are in excellent agreement with experiment "Anisotropic ball packing" proposed here plays an intermediate role between the enthalpy-favored "disk packing" and entropy-favored "isotropic ball packing", which explains the phase transitions at different temps. Free energies of various lattices at different densities are essentially the same, indicating that the preferred lattice is not determined during the packing process. Both enthalpy and entropy decrease as the d. increases. Free energy change with volume shows two stable phases: the condensed phase and the isolated micelle phase. The interactions between the soft dendrimer balls are lattice dependent when described by a two-body potential because the soft ball self-adjusts its shape and interaction in different lattices. The shape of the free energy potential is similar to that of the "square shoulder potential". A model explaining the packing efficiency of ideal soft balls in various lattices is proposed in terms of geometrical consideration.

IT 186031-59-4
RL: PRP (Properties)
(thermodn. properties of self-assembled dendron liquid crystals in various lattices by atomistic simulation)
RN 186031-59-4 CAPLUS
CN Benzoic acid, 3,4,5-tris[[3,4,5-tris(dodecyloxy)phenyl]methoxy]- (CA INDEX NAME)



RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

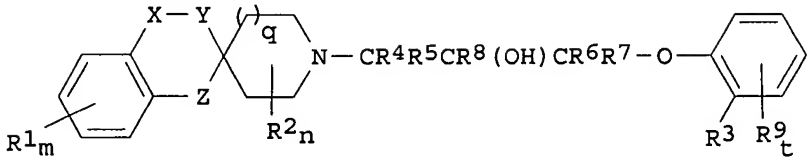
L15 ANSWER 30 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:41477 CAPLUS
DN 140:93937
TI Preparation of tricyclic spiropiperidines or spiropyrrolidines useful against disorders affected by modulation of chemokine receptors
IN Hossain, Nafizal; Ivanova, Svetlana; Mensonides-Harsema, Marguerite
PA Astrazeneca AB, Swed.
SO PCT Int. Appl., 281 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004005295	A1	20040115	WO 2003-SE1185	20030707
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2492122	A1	20040115	CA 2003-2492122	20030707
AU 2003243122	A1	20040123	AU 2003-243122	20030707
EP 1521757	A1	20050413	EP 2003-762957	20030707
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003012560	A	20050510	BR 2003-12560	20030707
CN 1675218	A	20050928	CN 2003-819146	20030707
JP 2005537255	T	20051208	JP 2004-519472	20030707

	NZ 537259	A	20060831	NZ 2003-537259	20030707
	CN 1974574	A	20070606	CN 2006-10143556	20030707
	IN 2004DN04014	A	20070427	IN 2004-DN4014	20041216
	ZA 2005000024	A	20060222	ZA 2005-24	20050103
	MX 2005PA00278	A	20050331	MX 2005-PA278	20050104
	US 2005245741	A1	20051103	US 2005-520699	20050107
	NO 2005000635	A	20050331	NO 2005-635	20050204
PRAI	SE 2002-2133	A	20020708		
	CN 2003-819146	A3	20030707		
	WO 2003-SE1185	W	20030707		

OS MARPAT 140:93937

GI



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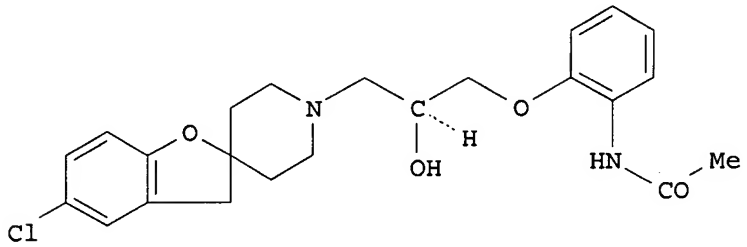


II

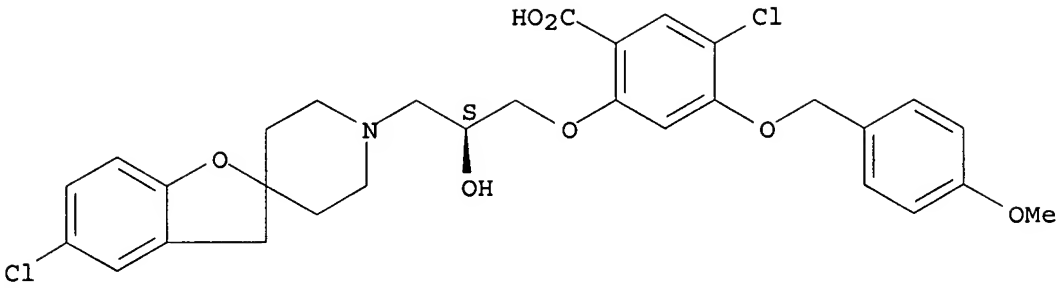
AB The invention provides tricyclic spiropiperidines or spiropyrrolidines (shown as I; variables defined below; e.g. II), processes for their preparation, pharmaceutical compns. containing them and their use in therapy for disorders affected by modulation of chemokine receptors (no data). For I: m is 0-4; each R1 = halogen, cyano, hydroxy, C1-C6 alkyl, C1-C6 haloalkyl, C1-C6 alkoxy or sulfonamido; either X = a bond, -CH2-, -O- or -C(O)- and Y = a bond, -CH2-, -O- or -C(O)-, or X and Y together = -CH:CMe- or -CMe:CH-, and Z = a bond, -O-, -NH- or -CH2-, provided that only one of X, Y and Z can be a bond at any one time and provided that X and Y do not both simultaneously = -O- or -C(O)-. N = 0-2; each R2 = halogen or C1-C6 alkyl; q = 0-1; R3 = -NHC(O)R10, -C(O)NR11R12 or -COOR12a; R4, R5, R6, R7 and R8 = H or a C1-C6 alkyl group; t = 0-2; each R9 = halogen, cyano, hydroxy, carboxy, C1-C6 alkoxy, C1-C6 alkoxycarbonyl, C1-C6 haloalkyl, or C1-C6 alkyl; addnl. details are given in the claims. Methods of preparation are claimed and >200 example prepns. are included. For example, II was prepared in 2 steps starting from N-(2-hydroxyphenyl)acetamide, ((2S)-oxiran-2-yl)methyl and Cs2CO3 in DMF to give N-[2-[((2S)-oxiran-2-yl)methoxy]phenyl]acetamide as an intermediate, which was reacted with 5-chloro-3H-spiro[1-benzofuran-2,4'-piperidine] in EtOH to give II.

IT 644971-09-5P 644971-47-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of tricyclic spiropiperidines or spiropyrrolidines useful against disorders affected by modulation of chemokine receptors)

RN 644971-09-5 CAPLUS

CN Benzoic acid, 5-chloro-2-[(2S)-3-(5-chlorospiro[benzofuran-2(3H),4'-piperidin]-1'-yl)-2-hydroxypropoxy]-4-[(4-methoxyphenyl)methoxy]-, hydrochloride (9CI) (CA INDEX NAME)

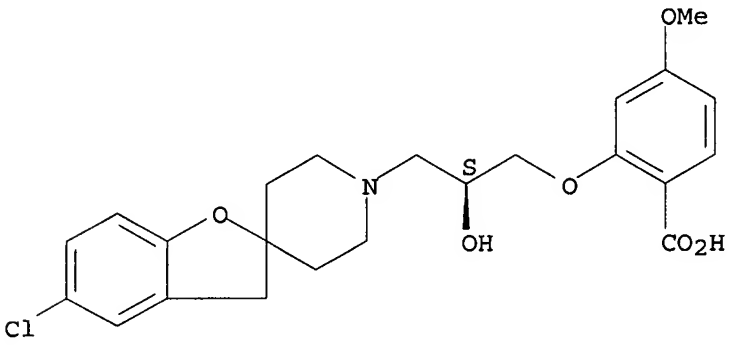
Absolute stereochemistry.



● HCl

RN 644971-47-1 CAPLUS
CN Benzoic acid, 2-[(2S)-3-(5-chlorospiro[benzofuran-2(3H),4'-piperidin]-1'-yl)-2-hydroxypropoxy]-4-methoxy-, hydrochloride (9CI) (CA INDEX NAME)

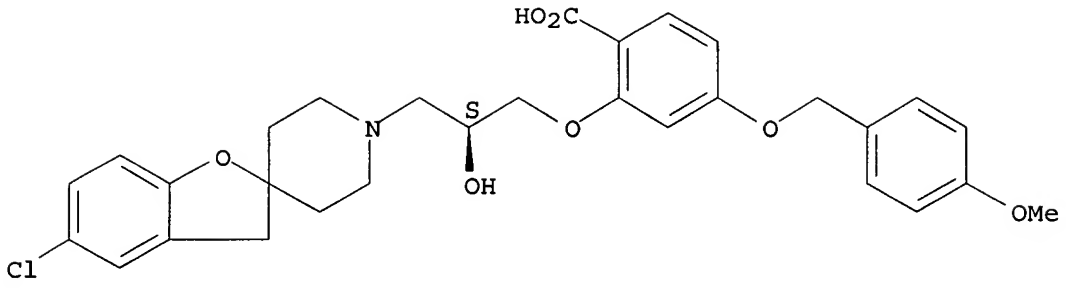
Absolute stereochemistry.



● HCl

IT 644970-97-8 644973-07-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of tricyclic spiropiperidines or spiropyrrolidines useful against disorders affected by modulation of chemokine receptors)
RN 644970-97-8 CAPLUS
CN Benzoic acid, 2-[(2S)-3-(5-chlorospiro[benzofuran-2(3H),4'-piperidin]-1'-yl)-2-hydroxypropoxy]-4-[(4-methoxyphenyl)methoxy]-, hydrochloride (9CI) (CA INDEX NAME)

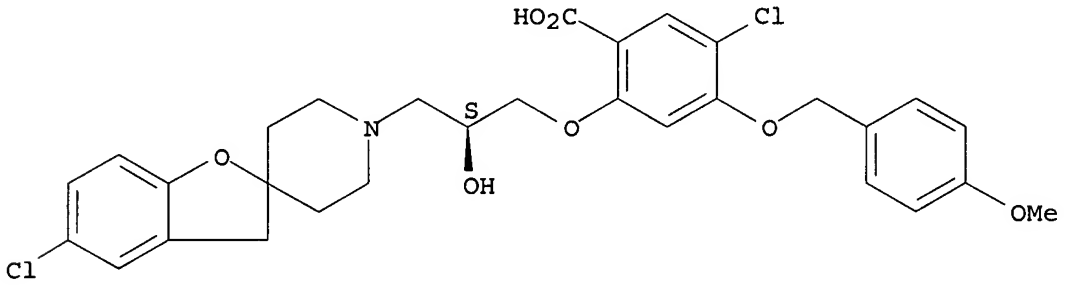
Absolute stereochemistry.



● HCl

RN 644973-07-9 CAPLUS
CN Benzoic acid, 5-chloro-2-[(2S)-3-(5-chlorospiro[benzofuran-2(3H),4'-piperidin]-1'-yl)-2-hydroxypropoxy]-4-[(4-methoxyphenyl)methoxy]- (9CI) (CA INDEX NAME)

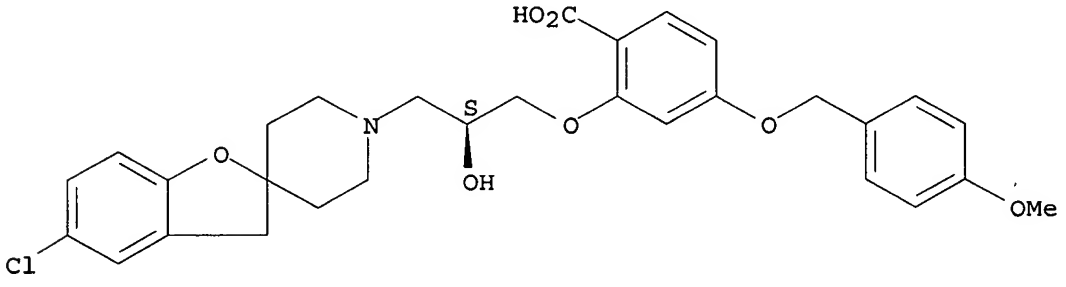
Absolute stereochemistry.



IT 644969-68-6P 644970-00-3P 644970-14-9P
644971-42-6P 644972-73-6P 644972-84-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tricyclic spiropiperidines or spiropyrrolidines useful against disorders affected by modulation of chemokine receptors)

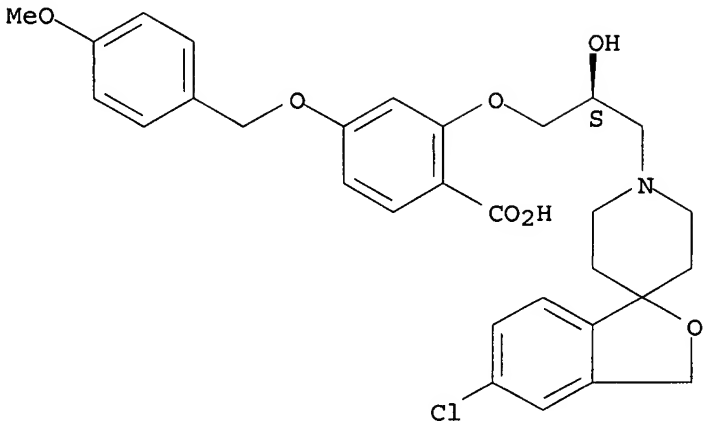
RN 644969-68-6 CAPLUS
CN Benzoic acid, 2-[(2S)-3-(5-chlorospiro[benzofuran-2(3H),4'-piperidin]-1'-yl)-2-hydroxypropoxy]-4-[(4-methoxyphenyl)methoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 644970-00-3 CAPLUS
CN Benzoic acid, 2-[(2S)-3-(5-chlorospiro[isobenzofuran-1(3H),4'-piperidin]-1'-yl)-2-hydroxypropoxy]-4-[(4-methoxyphenyl)methoxy]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

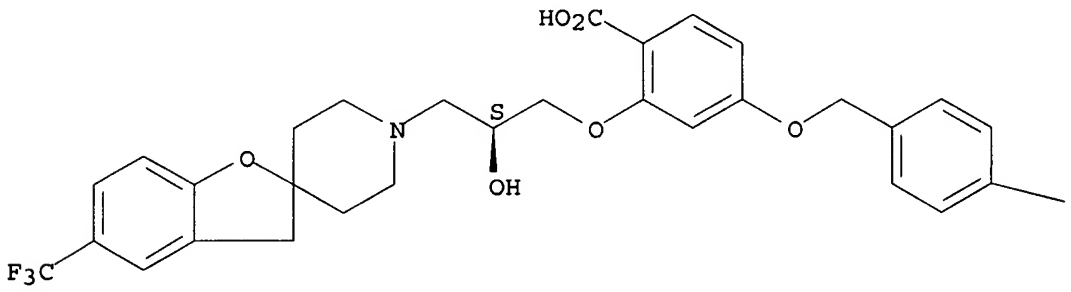


● HCl

RN 644970-14-9 CAPLUS
CN Benzoic acid, 2-[(2S)-2-hydroxy-3-[5-(trifluoromethyl)spiro[benzofuran-2(3H),4'-piperidin]-1'-yl]propoxy]-4-[(4-methoxyphenyl)methoxy]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● HCl

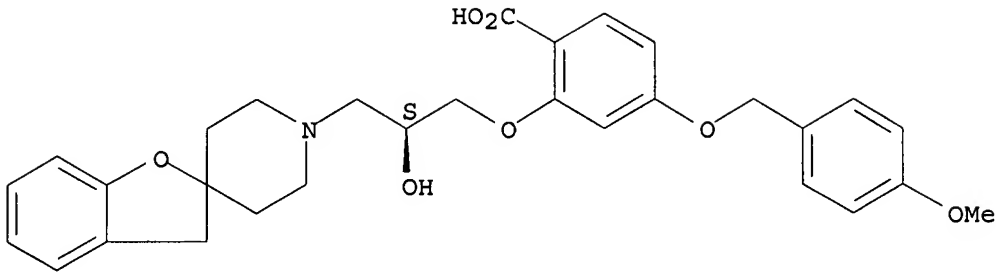
PAGE 1-B

OMe

RN 644971-42-6 CAPLUS
CN Benzoic acid, 2-[(2S)-2-hydroxy-3-spiro[benzofuran-2(3H),4'-piperidin]-1'-ylpropoxy]-4-[(4-methoxyphenyl)methoxy]-, hydrochloride (9CI) (CA INDEX

NAME)

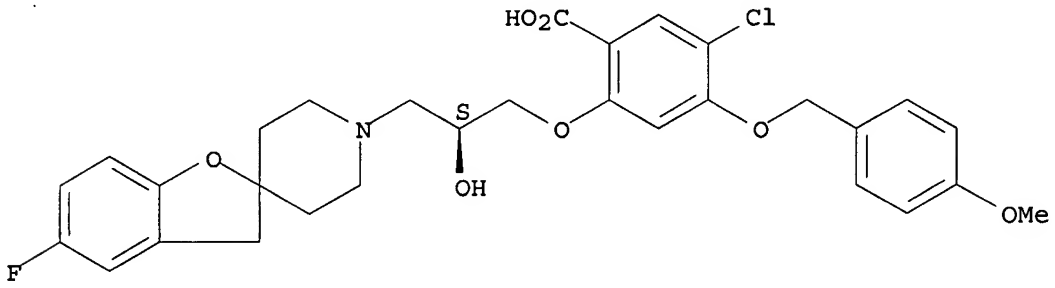
Absolute stereochemistry.



● HCl

RN 644972-73-6 CAPLUS
CN Benzoic acid, 5-chloro-2-[(2S)-3-(5-fluorospiro[benzofuran-2(3H),4'-piperidin]-1'-yl)-2-hydroxypropoxy]-4-[(4-methoxyphenyl)methoxy]-, hydrochloride (9CI) (CA INDEX NAME)

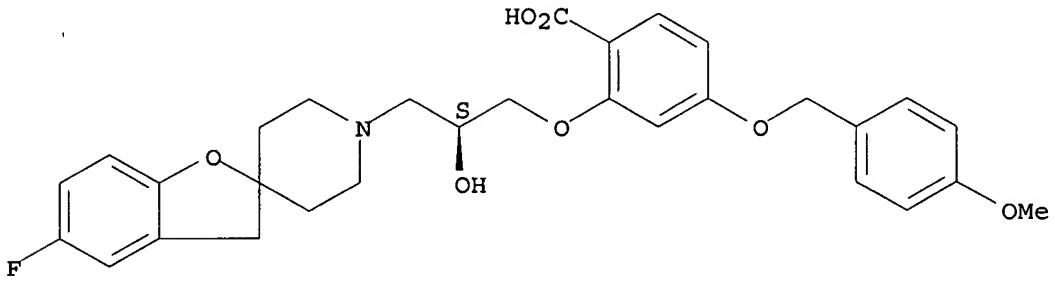
Absolute stereochemistry.



● HCl

RN 644972-84-9 CAPLUS
CN Benzoic acid, 2-[(2S)-3-(5-fluorospiro[benzofuran-2(3H),4'-piperidin]-1'-yl)-2-hydroxypropoxy]-4-[(4-methoxyphenyl)methoxy]-, hydrochloride (9CI) (CA INDEX NAME)

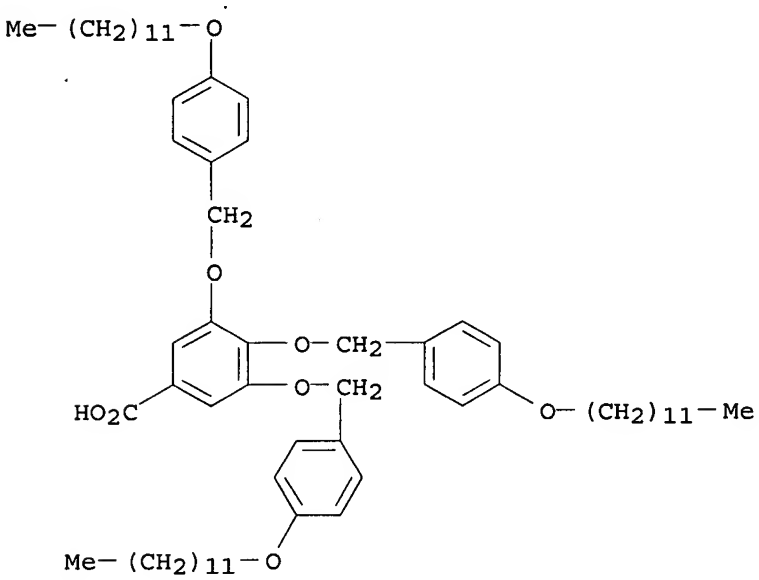
Absolute stereochemistry.



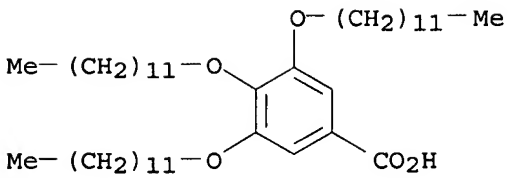
● HCl

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 31 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:1011359 CAPLUS
DN 140:205552
TI Surface Orientation of 3,4,5-Tris-Substituted Benzoic Acid Amphiphiles
AU Mourran, Ahmed; Beginn, Uwe; Zipp, Gabriela; Moeller, Martin
CS ITMC/DWI, RWTH Aachen, Aachen, D-52056, Germany
SO Langmuir (2004), 20(3), 673-679
CODEN: LANGD5; ISSN: 0743-7463
PB American Chemical Society
DT Journal
LA English
AB Regarding the mol. orientation on flat substrates, thin films have been studied of a series of wedge-shaped mols. (3,4,5-tris-substituted benzoate-benzo crown ether compds.) consisting of a hydrophobic outer rim and a polar group at the thin end which form columnar mesomorphic and crystalline structures. For most substrates studied here, autophobic dewetting is demonstrated to be caused by the formation of a monomol. adlayer in which the mols. are oriented normal to the substrate surface with the hydrophobic tails directed away from the substrate. For thick films, this adlayer is shown to cause an "in-plane" orientation of the axis of the columnar state. An ordered in-plane oriented adlayer is observed only for highly ordered pyrolytic graphite as the substrate. In this case, specific interactions with the substrate cause formation of a well-ordered 2D pattern that might favor homeotropic orientation of the columnar structures but has to be optimized by further structural variation. The structure of the adsorbed monolayer is elucidated by combining contact angle measurements, plasmon resonance spectroscopy, and optical and scanning tunneling microscopy.
IT 110934-58-2, 3,4,5-Tris[4-(dodecyloxy)benzyloxy]benzoic acid
117241-31-3, 3,4,5-Tridodecyloxybenzoic acid
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process)
(surface orientation of substituted benzoic acid amphiphiles)
RN 110934-58-2 CAPLUS
CN Benzoic acid, 3,4,5-tris[[4-(dodecyloxy)phenyl]methoxy]- (CA INDEX NAME)



RN 117241-31-3 CAPLUS
CN Benzoic acid, 3,4,5-tris(dodecyloxy)- (CA INDEX NAME)

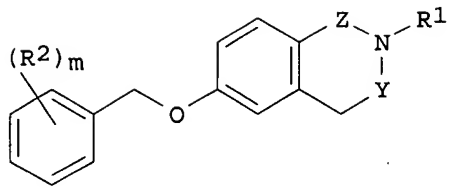


RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 32 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:875255 CAPLUS
DN 139:364839
TI Preparation of isoquinolines as monoamine oxidase B inhibitors useful against Alzheimer's disease and senile dementia
IN Cesura, Andrea; Rodriguez Sarmiento, Rosa Maria; Scalone, Michelangelo; Thomas, Andrew William; Wyler, Rene
PA F. Hoffmann-La Roche Ag, Switz.
SO PCT Int. Appl., 81 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003091219	A1	20031106	WO 2003-EP3845	20030414
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2483461	A1	20031106	CA 2003-2483461	20030414
	AU 2003227614	A1	20031110	AU 2003-227614	20030414
	EP 1501804	A1	20050202	EP 2003-725018	20030414
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	BR 2003009562	A	20050215	BR 2003-9562	20030414
	CN 1649844	A	20050803	CN 2003-809376	20030414
	JP 2005533761	T	20051110	JP 2003-587782	20030414
	NZ 535885	A	20070531	NZ 2003-535885	20030414
	US 2003225122	A1	20031204	US 2003-417378	20030416
	US 6818774	B2	20041116		
	ZA 2004008281	A	20051014	ZA 2004-8281	20041013
	NO 2004004571	A	20041022	NO 2004-4571	20041022
	MX 2004PA10537	A	20050125	MX 2004-PA10537	20041025
	IN 2004CN02409	A	20070427	IN 2004-CN2409	20041025
	HK 1080836	A1	20070629	HK 2006-100541	20060113
PRAI	EP 2002-9253	A	20020426		
	WO 2003-EP3845	W	20030414		

OS MARPAT 139:364839
GI



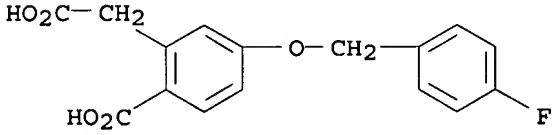
I

AB This invention relates to isoquinolines (shown as I; e.g. 2-[6-(3-fluorobenzyloxy)-1-oxo-3,4-dihydro-1H-isoquinolin-2-yl]acetamide; Y is C:O, or CH2; Z is C:O or CH2; R1 is H or CR3R4R5 (R3 is -(CH2)nC(O)NR6R7, -(CH2)nCOOR8, -CHR9COOR8, -(CH2)nCN, -(CH2)pOR8, -(CH2)nNR6R7, -(CH2)nCF3, -(CH2)nNHC(O)R9, -(CH2)nNHCOOR8, -(CH2)ntetrahydrofuranyl, -(CH2)pSR8, -(CH2)pS(O)R9, or -(CH2)nC(S)NR5R6; R4 is H, C1-C6-alkyl, - (CH2)pOR8, -(CH2)pSR8, or benzyl; R5 is H, C1-C6-alkyl, -(CH2)pOR8, -(CH2)pSR8, or benzyl; R6 and R7 = H or C1-C6-alkyl; R8 is H or C1-C6-alkyl; R9 is C1-C6-alkyl; m = 1-3; n = 0-2; and p = 1-2; R2 = halogen, halogen-(C1-C6)-alkyl, cyano, C1-C6-alkoxy or halogen-(C1-C6)-alkoxy)) as well as to their pharmaceutically acceptable salts. The invention further relates to medicaments containing these compds., a process for their preparation as well as their use for preparation of medicaments for the treatment or prevention of diseases in which MAO-B inhibitors might be beneficial. IC50 values for 17 examples of I against monoamine oxidase A and B are tabulated, e.g. 0.008 and 0.33 μM for 2-[6-(3-fluorobenzyloxy)-1-oxo-3,4-dihydro-1H-isoquinolin-2-yl]acetamide. Sixty example prepns. of I are included. For example, 6-(3-Fluorobenzyloxy)-3,4-dihydro-2H-isoquinolin-1-one was prepared in 3 steps (49, 65, 87 % yields) starting from 5-methoxy-1-indanone and involving intermediates 6-methoxy-3,4-dihydro-2H-isoquinolin-1-one and 6-hydroxy-3,4-dihydro-2H-isoquinolin-1-one.

IT 620607-00-3P, 2-(Carboxymethyl)-4-(4-fluorobenzyloxy)benzoic acid
620607-02-5P, 4-(4-Fluorobenzyloxy)-2-[(methoxycarbonyl)methyl]benzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoquinolines as monoamine oxidase B inhibitors useful against Alzheimer's disease and senile dementia)

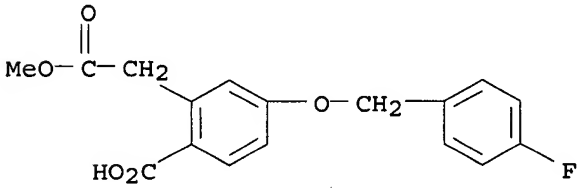
RN 620607-00-3 CAPLUS

CN Benzeneacetic acid, 2-carboxy-5-[(4-fluorophenyl)methoxy]- (9CI) (CA INDEX NAME)



RN 620607-02-5 CAPLUS

CN Benzeneacetic acid, 2-carboxy-5-[(4-fluorophenyl)methoxy]-, α-methyl ester (9CI) (CA INDEX NAME)

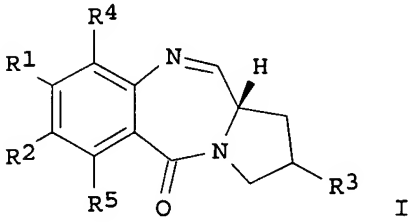


RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 33 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:777438 CAPLUS
DN 139:292092
TI Synthesis of pyrrolo[2,1-c][1,4]benzodiazepine analogs
IN Wang, Jeh-Jeng
PA Kaohsiung Medical University, Taiwan
SO U.S. Pat. Appl. Publ., 12 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2003187253	A1	20031002	US 2002-94140	20020308
US 6660856	B2	20031209		
PRAI US 2002-94140		20020308		

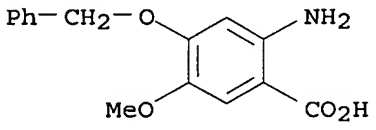
OS CASREACT 139:292092; MARPAT 139:292092
GI



I

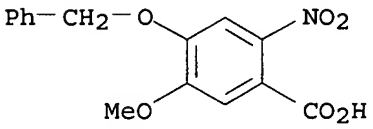
AB The present invention provides an efficient process for the preparation of pyrrolo[2,1-c][1,4]benzodiazepines (PBDS) I (R1, R2 = H, halo, amino, cyano, HO, NO2, phenoxy, C1-12-alkyl, C1-12-alkoxy, C1-12-alkenoxy which may be optionally substituted; R3 = H, alkyl, alkenyl, alkenylidene, HO, alkoxy; R4, R5 = H, halo, cyano, HO, phenoxy, C1-8-alkyl, C1-6-alkoxy which may be optionally substituted) were prepared starting from a substituted 2-aminobenzoic acid derivative, and involves a step of reduction of an intermediate MOM-protected dilactam compound in the presence of LiBH4. The process enables a practical and large scale (e.g., ca. 10 g) synthesis of PBD analogs. Thus, DC-81 was prepared in 6 steps starting from 4-benzyloxy-5-methoxy-2-nitrobenzoic acid.

IT 155666-33-4P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of pyrrolo[2,1-c][1,4]benzodiazepine analogs)
RN 155666-33-4 CAPLUS
CN Benzoic acid, 2-amino-5-methoxy-4-(phenylmethoxy)- (CA INDEX NAME)



IT 60547-92-4, 4-Benzyloxy-5-methoxy-2-nitrobenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of pyrrolo[2,1-c][1,4]benzodiazepine analogs)

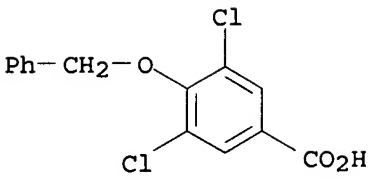
RN 60547-92-4 CAPLUS
CN Benzoic acid, 5-methoxy-2-nitro-4-(phenylmethoxy)- (CA INDEX NAME)



L15 ANSWER 34 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:532632 CAPLUS
DN 139:99939
TI Agaricoglycerides produced by Basidiomycetes and their analogs
IN Stadler, Marc; Hellwig, Veronika; Wiese, Burkhardt; Burkhardt, Nils; Denzer, Dirk; Mayer-Bartschmid, Anke; Allerheiligen, Swen; Gerisch, Michael; Wirtz, Stephan-Nicholas
PA Bayer Aktiengesellschaft, Germany
SO PCT Int. Appl., 147 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003055843	A1	20030710	WO 2002-EP14289	20021216
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	DE 10238007	A1	20030710	DE 2002-10238007	20020820
	AU 2002358719	A1	20030715	AU 2002-358719	20021216
PRAI	DE 2001-10164141	A	20011227		
	DE 2002-10238007	A	20020820		
	WO 2002-EP14289	W	20021216		

OS MARPAT 139:99939
AB The invention relates to agaricoglycerides and analogs, methods for the production thereof, in addition to the use thereof for the production of medicaments for treating and/or the prophylaxis of illnesses, especially painful conditions.
Thus, agaricoglycerides A and B were isolated from the wet mycelia of Agaricus strain WP 4080.
IT 41490-13-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(agaricoglycerides produced by Basidiomycetes and their analogs)
RN 41490-13-5 CAPLUS
CN Benzoic acid, 3,5-dichloro-4-(phenylmethoxy)- (CA INDEX NAME)

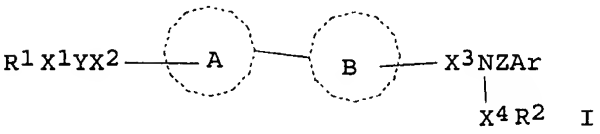


RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 35 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:539647 CAPLUS
DN 137:109128
TI Preparation of biaryl compounds for treatment of hyperlipidemia and arteriosclerosis
IN Kori, Masakuni; Ishikawa, Eiichiro; Nakata, Mikiyo; Kobayashi, Makoto
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 470 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002055484	A1	20020718	WO 2002-JP73	20020110
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2002226675	A1	20020724	AU 2002-226675	20020110
	JP 2003055326	A	20030226	JP 2002-4422	20020111
PRAI	JP 2001-5823	A	20010112		
	JP 2001-174901	A	20010608		
	WO 2002-JP73	W	20020110		

OS MARPAT 137:109128
GI

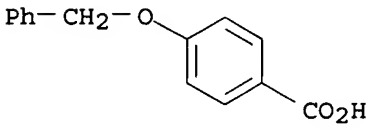


AB The title compds. I [rings A and B each represents an optionally substituted five- or six-membered aromatic ring; R1 and R2 each represents hydrogen, an optionally substituted hydrocarbon group, or an optionally substituted heterocyclic group; X1, X2, X3, and X4 each represents a bond or an optionally substituted divalent hydrocarbon group; Y represents NR3CO, CONR3, NR3SO2, SO2NR3, NR3CH2 (R3 represents hydrogen, an optionally substituted hydrocarbon group, or an optionally substituted heterocyclic group), etc.; Z represents CONH, CSNH, CO, or SO2; and Ar represents an optionally substituted cyclic hydrocarbon group or an optionally substituted heterocyclic group] are prepared I increase the amount of low-d. lipoprotein (LDL) receptors. The LDL receptor gene transcription promoting activities of compds. of this invention were

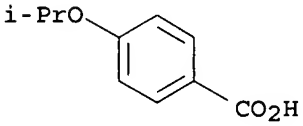
demonstrated. Processes for preparing I are disclosed.

IT 1486-51-7, 4-Benzyloxybenzoic acid 13205-46-4, 4-Isopropoxybenzoic acid 30762-00-6, 4-Isobutoxybenzoic acid 177025-66-0, 4-Cyclohexylmethoxybenzoic acid 355391-06-9 443345-84-4 443345-85-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of biaryl compds. for treatment of hyperlipidemia and arteriosclerosis)

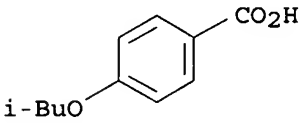
RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



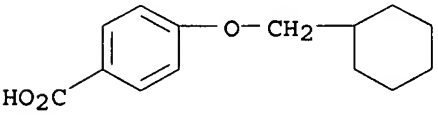
RN 13205-46-4 CAPLUS
CN Benzoic acid, 4-(1-methylethoxy)- (CA INDEX NAME)



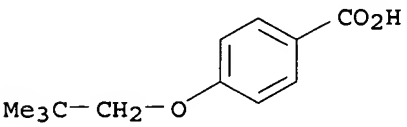
RN 30762-00-6 CAPLUS
CN Benzoic acid, 4-(2-methylpropoxy)- (CA INDEX NAME)



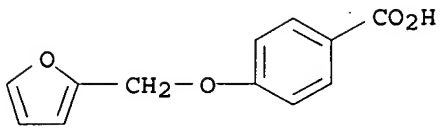
RN 177025-66-0 CAPLUS
CN Benzoic acid, 4-(cyclohexylmethoxy)- (9CI) (CA INDEX NAME)



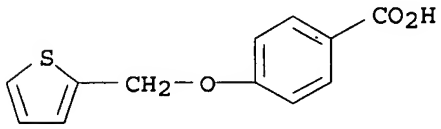
RN 355391-06-9 CAPLUS
CN Benzoic acid, 4-(2,2-dimethylpropoxy)- (9CI) (CA INDEX NAME)



RN 443345-84-4 CAPLUS
CN Benzoic acid, 4-(2-furanylmethoxy)- (9CI) (CA INDEX NAME)



RN 443345-85-5 CAPLUS
CN Benzoic acid, 4-(2-thienylmethoxy)- (9CI) (CA INDEX NAME)

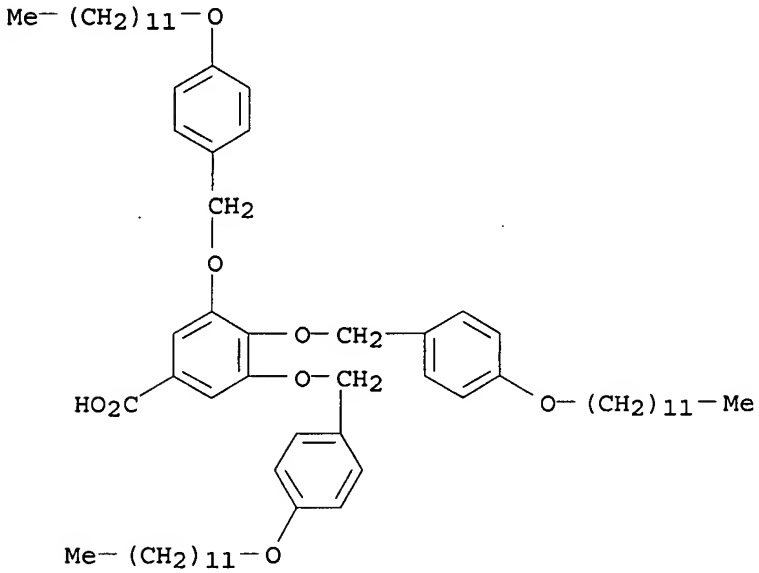


RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

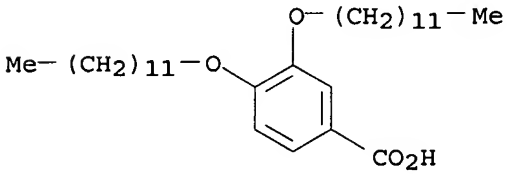
L15 ANSWER 36 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:386021 CAPLUS
DN 137:294947
TI Synthesis and NaOTf mediated self-assembly of monodendritic crown ethers
AU Percec, Virgil; Cho, Wook-Dong; Ungar, Goran; Yeardley, Duncan J. P.
CS Roy & Diana Vagelos Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104-6323, USA
SO Chemistry--A European Journal (2002), 8(9), 2011-2025
CODEN: CEUJED; ISSN: 0947-6539
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
OS CASREACT 137:294947
AB The synthesis of ten benzyl ether based self-assembling monodendrons containing benzo[15]crown-5 at their focal point is presented. These dendritic building blocks self-assemble either directly or via complexation with NaOTf in two-dimensional smectic B, smectic A, and p6mm hexagonal columnar and three-dimensional Pm.hivin.3n cubic lattices. Retro-structural anal. of these lattices and of the lattices generated from the same monodendrons containing various other functional groups at their focal point by X-ray diffraction expts. provided for the first time a correlation between the mol. structure and the shape of the monodendron, the shape of the supramol. dendrimer and the symmetry of the lattice. It was shown that complexation with NaOTf provides the following five different trends: (a) stabilization of the three-dimensional Pm.hivin.3n cubic lattice self-organized from spherical dendrimers that are self-assembled from conic monodendrons; (b) stabilization of the two-dimensional SA phase generated from parallelepiped monodendrons; (c) no effect on the stability of the two-dimensional SB phase generated from parallelepiped monodendrons; (d) stabilization of the two-dimensional p6mm hexagonal columnar phase self-organized from cylindrical supramol. dendrimers that are self-assembled from tapered monodendrons; and (e) destabilization of the two-dimensional p6mm hexagonal columnar phase self-organized from cylindrical supramol. dendrimers self-assembled from half-disk monodendrons. Mechanisms of NaOTf mediated self-assembly processes were suggested. These monodendritic crown ethers and their NaOTf complexes provide the largest diversity of liquid crystalline phases encountered so far in any library of supramol. dendrimers.
IT 110934-58-2, 3,4,5-Tris[[4-(dodecyloxy)phenyl]methoxy]benzoic acid 131525-58-1, 3,4-Bis(dodecyloxy)benzoic acid 186031-59-4, 3,4,5-Tris[[3,4,5-tris(dodecyloxy)phenyl]methoxy]benzoic acid 212627-81-1, 3,4-Bis[[4-(dodecyloxy)phenyl]methoxy]benzoic acid 212627-86-6, 3,4-Bis[[3,4-bis(dodecyloxy)phenyl]methoxy]benzoic

acid 212627-88-8, 3,4,5-Tris[[3,4-bis(dodecyloxy)phenyl]methoxy]
benzoic acid 331822-46-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and sodium triflate-mediated self-assembly of monodendritic
crown ethers)

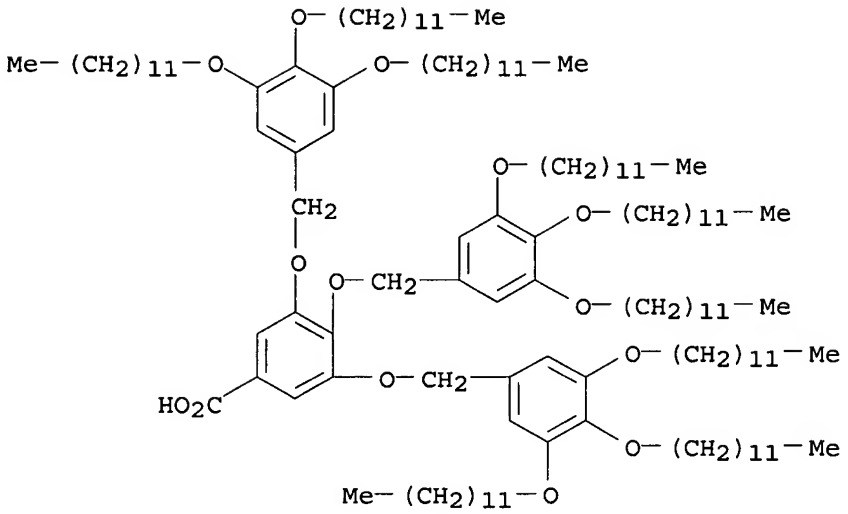
RN 110934-58-2 CAPLUS
CN Benzoic acid, 3,4,5-tris[[4-(dodecyloxy)phenyl]methoxy]- (CA INDEX NAME)



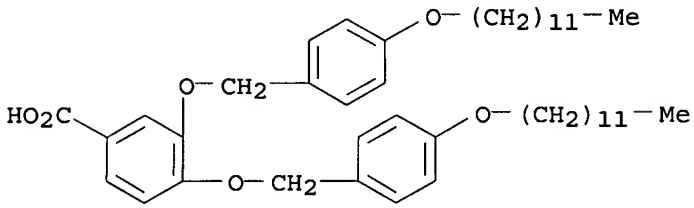
RN 131525-58-1 CAPLUS
CN Benzoic acid, 3,4-bis(dodecyloxy)- (CA INDEX NAME)



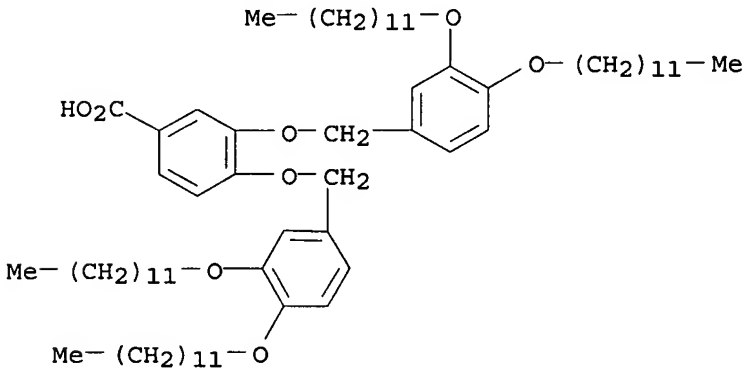
RN 186031-59-4 CAPLUS
CN Benzoic acid, 3,4,5-tris[[3,4,5-tris(dodecyloxy)phenyl]methoxy]- (CA
INDEX NAME)



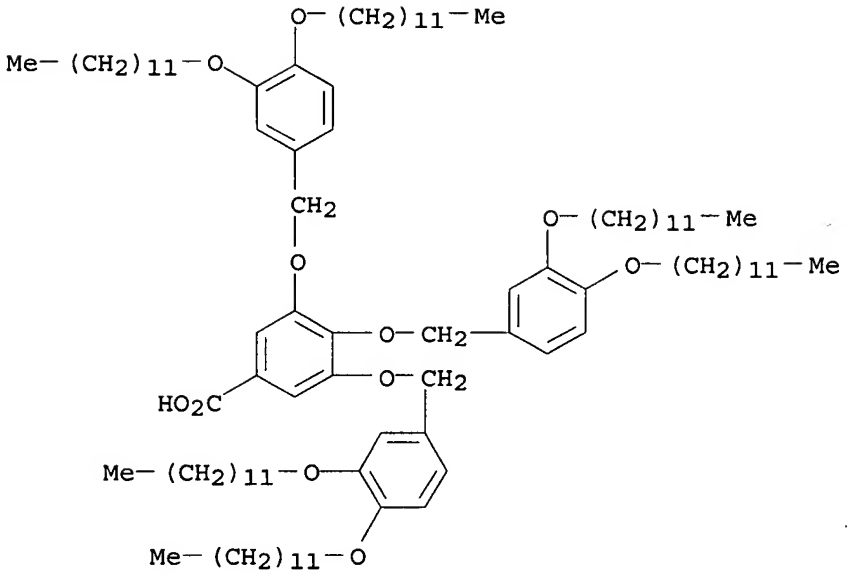
RN 212627-81-1 CAPLUS
CN Benzoic acid, 3,4-bis[[4-(dodecyloxy)phenyl]methoxy]- (9CI) (CA INDEX NAME)



RN 212627-86-6 CAPLUS
CN Benzoic acid, 3,4-bis[[3,4-bis(dodecyloxy)phenyl]methoxy]- (9CI) (CA INDEX NAME)

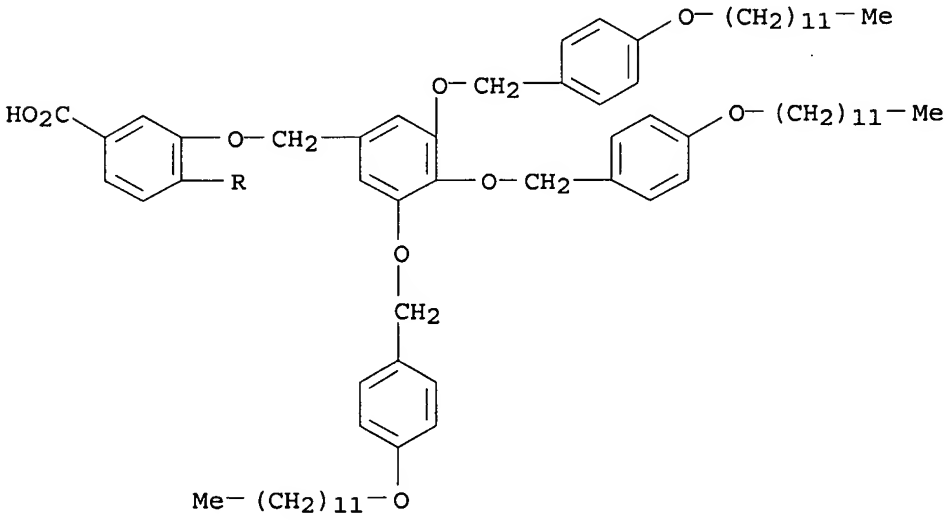


RN 212627-88-8 CAPLUS
CN Benzoic acid, 3,4,5-tris[[3,4-bis(dodecyloxy)phenyl]methoxy]- (9CI) (CA INDEX NAME)

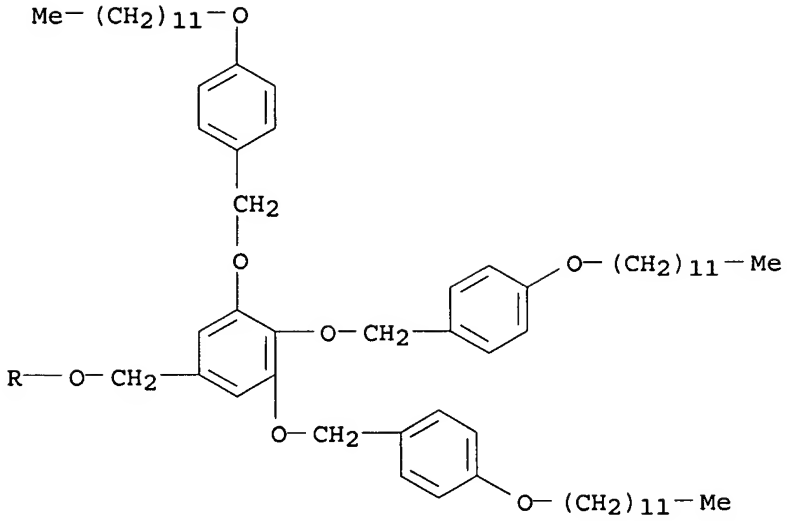


RN 331822-46-9 CAPLUS
CN Benzoic acid, 3,4-bis[[3,4,5-tris[[4-(dodecyloxy)phenyl]methoxy]phenyl]methoxy]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

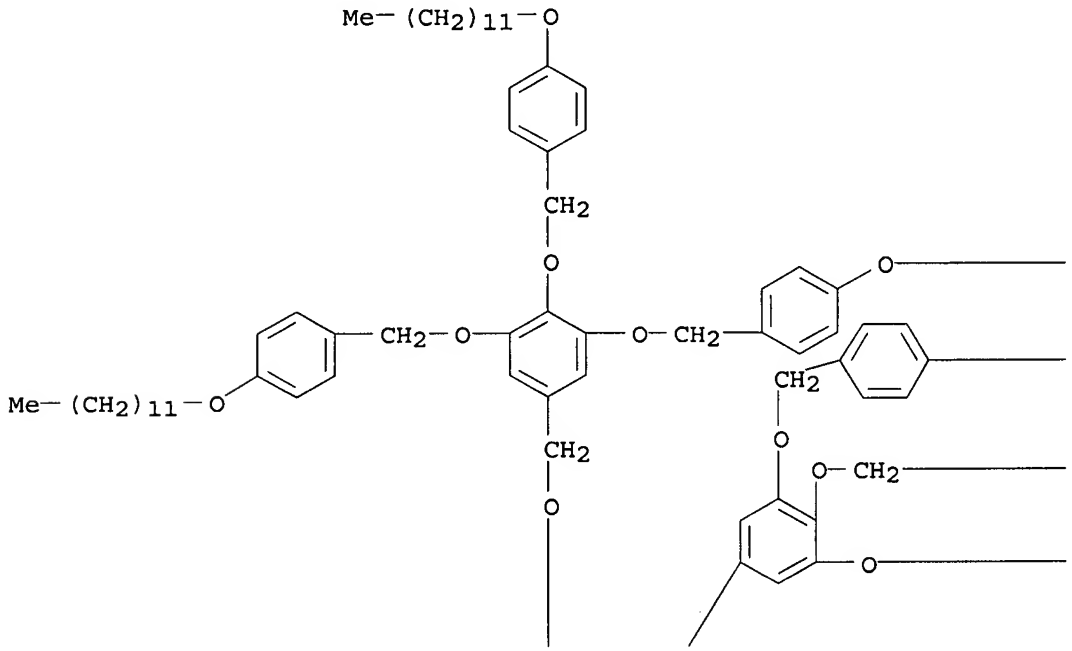


IT 469905-74-6P, 3,4,5-Tris[[3,4,5-tris[[4-(dodecyloxy)phenyl]methoxy]phenyl]methoxy]benzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and sodium triflate-mediated self-assembly of monodendritic crown ethers)

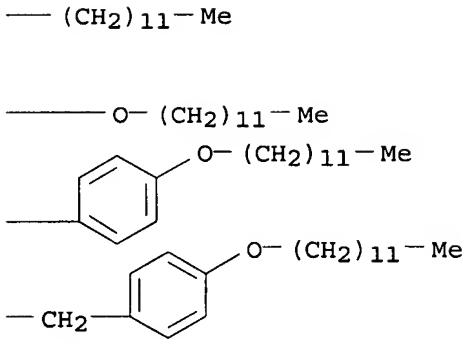
RN 469905-74-6 CAPLUS

CN Benzoic acid, 3,4,5-tris[[3,4,5-tris[[4-(dodecyloxy)phenyl]methoxy]phenyl]methoxy]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



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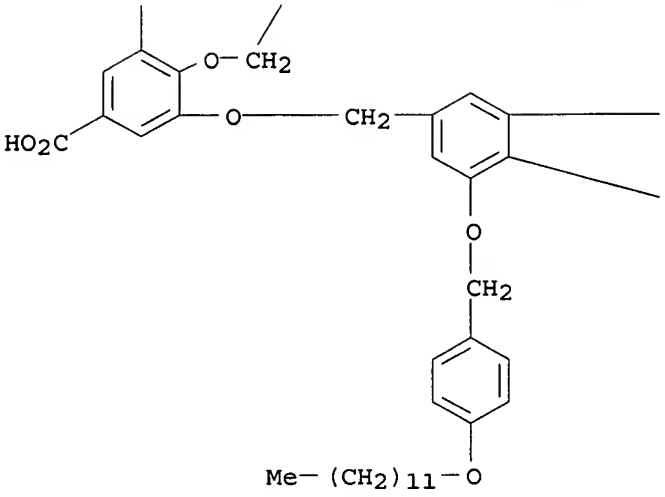
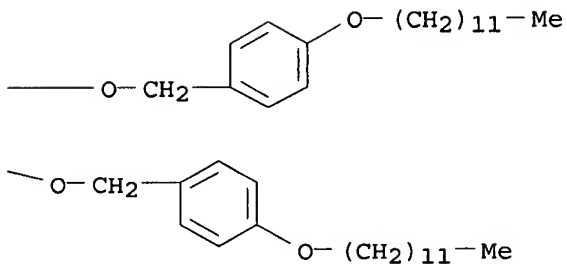


PAGE 2-B



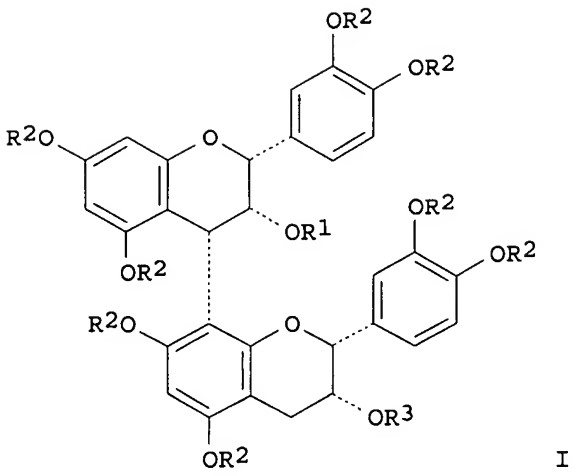
RE.CNT 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 37 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:185102 CAPLUS
DN 136:247439
TI Process for preparing 4α-aryl substituted epicatechin derivatives
IN Kozikowski, Alan P.; Romanczyk, Leo J., Jr.; Tueckmantel, Werner
PA Mars, Inc., USA
SO PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002020506	A2	20020314	WO 2001-US26175	20010821
	WO 2002020506	A3	20030206		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 6476241	B1	20021105	US 2000-655360	20000905
	CA 2421513	A1	20020314	CA 2001-2421513	20010821
	AU 200183472	A	20020322	AU 2001-83472	20010821
	EP 1317437	A2	20030611	EP 2001-962277	20010821
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004508362	T	20040318	JP 2002-525127	20010821
	RU 2281942	C2	20060820	RU 2003-109618	20010821
	AU 2001283472	B2	20070524	AU 2001-283472	20010821
	US 2003100775	A1	20030529	US 2002-214830	20020808
	US 6720432	B2	20040413		
	US 2005014958	A1	20050120	US 2004-783801	20040220
	US 7126014	B2	20061024		
	US 2007197804	A1	20070823	US 2006-543415	20061005
PRAI	US 2000-655360	A	20000905		
	WO 2001-US26175	W	20010821		
	US 2001-655360	A3	20010905		
	US 2002-214830	A3	20020808		
	US 2004-783801	A3	20040220		

OS CASREACT 136:247439; MARPAT 136:247439
GI



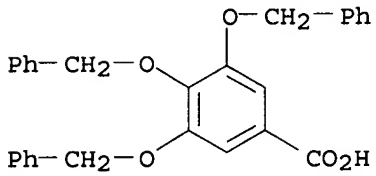
I

AB Process for preparing a 4α-aryl substituted epicatechin derivative including 4α,8-epicatechin dimers such as I (R1,R3 = H, acetyl, protected galloyl, galloyl; R2 = H, benzyl, acetyl), is disclosed which comprises the steps of: (a) protecting C-3 hydroxyl group of 5,7,3',4'-tetra-O-benzylepicatechin; (b) oxidizing the 4-position of the compound of step (a) to produce protected flavan-4-one; (c) reacting the compound of step (b) with aryllithium reagents, derived by halogen/metal exchange from the aryl bromides, to form C-3 protected 4-hydroxy-4-aryl epicatechin derivative; (d) deoxygenating the C-4 position of the compound of step (c) with tri-n-butyltin hydride and trifluoroacetic acid, to afford C-3 protected 4α-aryl-5,7,3',4'-tetra-O-benzylepicatechin. Thus, epicatechin-4α,8-(3-O-galloylepicatechin) I (R1, R2 = H; R3 = galloyl) was prepared in a multistep synthetic sequence starting from 5,7,3',4'-tetra-O-benzylepicatechin, 5,7,3',4'-tetra-O-benzyl-8-bromoepicatechin, and tri-O-benzyl gallic acid.

IT 1486-48-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(methods for the preparation of 4α-aryl substituted epicatechin derivs.)

RN 1486-48-2 CAPLUS

CN Benzoic acid, 3,4,5-tris(phenylmethoxy)- (CA INDEX NAME)



L15 ANSWER 38 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:116940 CAPLUS

DN 137:149777

TI Differential Inhibition of Polymerase and Strand-Transfer Activities of HIV-1 Reverse Transcriptase

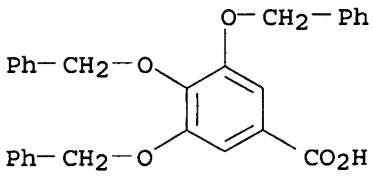
AU Tillekeratne, L. M. Viranga; Sherette, Angela; Fulmer, Jennifer A.; Hupe, Lynn; Hupe, Donald; Gabbara, Sam; Peliska, James A.; Hudson, Richard A.

CS Department of Medicinal and Biological Chemistry, University of Toledo, College of Pharmacy, Toledo, OH, 43606, USA

SO Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 525-528
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal
LA English
OS CASREACT 137:149777
AB A new class of inhibitors of HIV-1 reverse transcriptase obtained by the systematic structural simplification of epicatechin and epigallocatechin gallates are also shown here to inhibit DNA-strand-transfer, a process critical to the completion of the HIV-1-RT reproduction and to recombination-associated mutation of the virus. Up to 80-fold selectivity for DNA-strand-transfer inhibition over polymerase inhibition was observed for a defined subset of these agents. Such specific DNA-strand-transfer inhibitors may have important therapeutic potential.
IT 1486-48-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(differential inhibition of polymerase and strand-transfer activities of HIV-1 reverse transcriptase by compds. structurally related to epicatechin and epigallocatechin gallates)
RN 1486-48-2 CAPLUS
CN Benzoic acid, 3,4,5-tris(phenylmethoxy)- (CA INDEX NAME)



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 39 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:904160 CAPLUS
DN 136:20087
TI Preparation of 4-anilinoquinazoline derivatives for the treatment of tumors
IN Hennequin, Laurent Francois Andre; Ple, Patrick
PA Astrazeneca Ab, Swed.; Astrazeneca Uk Limited
SO PCT Int. Appl., 234 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001094341	A1	20011213	WO 2001-GB2424	20010601
	WO 2001094341	A9	20030417		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2407371	A1	20011213	CA 2001-2407371	20010601
	EP 1292594	A1	20030319	EP 2001-934176	20010601
	EP 1292594	B1	20040901		
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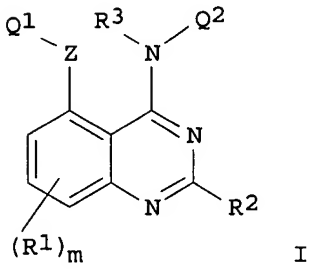
	BR 2001011335	A	20030610	BR 2001-11335	20010601
	HU 200301046	A2	20030828	HU 2003-1046	20010601

	JP 2003535859	T	20031202	JP 2002-501890	20010601
	JP 3774438	B2	20060517		
	EE 200200673	A	20040615	EE 2002-673	20010601
	NZ 522204	A	20040730	NZ 2001-522204	20010601
	AT 275145	T	20040915	AT 2001-934176	20010601
	PT 1292594	T	20041231	PT 2001-934176	20010601
	ES 2225545	T3	20050316	ES 2001-1934176	20010601
	RU 2276151	C2	20060510	RU 2002-135617	20010601
	IN 2002MN01457	A	20050304	IN 2002-MN1457	20021021
	US 2004214841	A1	20041028	US 2002-275382	20021105
	US 7049438	B2	20060523		
	ZA 2002009122	A	20040209	ZA 2002-9122	20021108
	MX 2002PA11765	A	20030410	MX 2002-PA11765	20021128
	BG 107332	A	20030731	BG 2002-107332	20021128
	NO 2002005792	A	20021202	NO 2002-5792	20021202
	HK 1053115	A1	20050408	HK 2003-105395	20030725
PRAI	EP 2000-401581	A	20000606		
	EP 2001-400297	A	20010207		
	EP 2001-400565	A	20010305		
	WO 2001-GB2424	W	20010601		

OS MARPAT 136:20087

GI



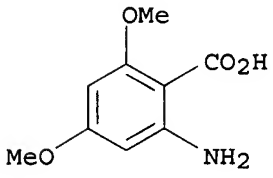
I

AB The invention concerns quinazoline derivs. (I; e.g. 4-(2-chloro-5-methoxyanilino)-7-methoxy-5-(3-morpholinopropoxy)quinazoline (1)), processes for their preparation, pharmaceutical compns. containing them and their use in the manufacture of a medicament for use as an anti-invasive agent in the containment and/or treatment of solid tumor disease. Although biol. assay methods are described, no test results are reported. It is believed that the antitumor activity is due to inhibition of one or more of the non-receptor tyrosine-specific protein kinases of the Src family that are involved in the signal transduction steps that lead to the invasiveness and migratory ability of metastasizing tumor cells. In I, according to the 1st claim, m = 0-3; each R1 = halo, trifluoromethyl, cyano, isocyano, nitro, hydroxy, mercapto, amino, formyl, carboxy, carbamoyl, (1-6C)alkyl, (2-8C)alkenyl, (2-8C)alkynyl, (1-6C)alkoxy, (2-6C)alkenyloxy, (2-6C)alkynyloxy, (1-6C)alkylthio, (1-6C)alkylsulfinyl, (1-6C)alkylsulfonyl, (1-6C)alkylamino, di[(1-6C)alkyl]amino, (1-6C)alkoxycarbonyl, N-(1-6C)alkylcarbamoyl, N,N-di[(1-6C)alkyl]carbamoyl, (2-6C)alkanoyl, (2-6C)alkanoyloxy, (2-6C)alkanoylamino, N-(1-6C)alkyl-(2-6C)alkanoylamino, (3-6C)alkenoylamino, N-(1-6C)alkyl-(3-6C)alkenoylamino, (3-6C)alkynoylamino, N-(1-6C)alkyl-(3-6C)alkynoylamino, N-(1-6C)alkylsulfamoyl, N,N-di[(1-6C)alkyl]sulfamoyl, (1-6C)alkanesulfonylamino and N-(1-6C)alkyl-(1-6C)alkanesulfonylamino, or Q3-X1- (X1 = direct bond, O, S, SO, SO2, N(R4), CO, CH(OR4), CON(R4), N(R4)CO, SO2N(R4), N(R4)SO2, OC(R4)2, SC(R4)2 and N(R4)C(R4)2 (R4 = H or (1-6C)alkyl) and Q3 = aryl, aryl-(1-6C)alkyl, (3-7C)cycloalkyl, (3-7C)cycloalkyl-, (1-6C)alkyl, (3-7C)cycloalkenyl, (3-7C)cycloalkenyl-(1-6C)alkyl, heteroaryl, heteroaryl-(1-6C)alkyl, heterocyclyl or heterocyclyl-(1-6C)alkyl), or (R1)m is (1-3C)alkylenedioxy, with addnl.

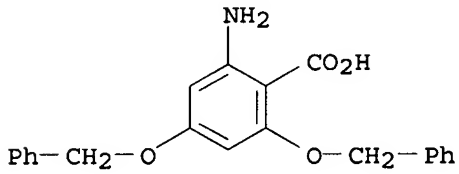
optional substitution and/or insertion possible. R2 = H or (1-6C)alkyl; R3 = H or (1-6C)alkyl; Z = direct bond, O, S, SO, SO2, N(R11), CO, CH(OR11), CON(R11), N(R11)CO, SO2N(R11), N(R11)SO2, OC(R11)2, SC(R11)2 and N(R11)C(R11)2 (R11 = H, or (1-6C)alkyl). Q1 = aryl, aryl-(1-6C)alkyl, (3-7C)cycloalkyl, (3-7C)cycloalkyl-(1-6C)alkyl, (3-7C)cycloalkenyl, (3-7C)cycloalkenyl-(1-6C)alkyl, heteroaryl, heteroaryl-(1-6C)alkyl, heterocyclyl or heterocyclyl-(1-6C)alkyl, or, when Z is a direct bond or O, Q1 may be (1-6C)alkyl, (2-8C)alkenyl, (2-8C)alkynyl, halo-(1-6C)alkyl, hydroxy-(1-6C)alkyl, (1-6C)alkoxy-(1-6C)alkyl, cyano-(1-6C)alkyl, amino-(1-6C)alkyl, (1-6C)alkylamino-(1-6C)alkyl, di[(1-6C)alkyl]amino-(1-6C)alkyl, (1-6C)alkylthio-(1-6C)alkyl, (1-6C)alkylsulfinyl-(1-6C)alkyl or (1-6C)alkylsulfonyl-(1-6C)alkyl, with addnl. optional substitution and/or insertion possible. Q2 = substituted Ph. More than 50 example prepns. are included. For example, 1 was obtained by adding di-tert-Bu azodicarboxylate (0.208 g) dropwise to a stirred mixture of 4-(2-chloro-5-methoxyanilino)-5-hydroxy-7-methoxyquinazoline (0.2 g), 4-(3-hydroxypropyl)morpholine, PPh3 (0.237 g) and CH2Cl2 (3 mL). The reaction mixture was stirred at ambient temperature for 1 h.

IT 21577-57-1P, 2-Amino-4,6-dimethoxybenzoic acid
379228-31-6P, 2-Amino-4,6-dibenzyloxybenzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of anilinoquinazoline derivs. for treatment of tumors)

RN 21577-57-1 CAPLUS
CN Benzoic acid, 2-amino-4,6-dimethoxy- (CA INDEX NAME)



RN 379228-31-6 CAPLUS
CN Benzoic acid, 2-amino-4,6-bis(phenylmethoxy)- (CA INDEX NAME)



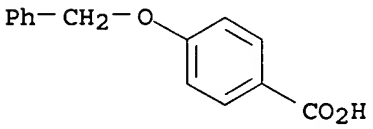
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 40 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:387279 CAPLUS
DN 135:138036
TI Antiferroelectric Liquid-Crystal Gels
AU Artal, M. Carmen; Ros, M. Blanca; Serrano, Jose Luis; de la Fuente, M. Rosario; Perez-Jubindo, Miguel Angel
CS Departamento de Quimica Organica Facultad de Ciencias-ICMA, Universidad de Zaragoza-CSIC, Zaragoza, 50009, Spain
SO Chemistry of Materials (2001), 13(6), 2056-2067
CODEN: CMATEX; ISSN: 0897-4756
PB American Chemical Society
DT Journal
LA English
AB The synthesis and characterization of several mesogenic antiferroelec.

gels-obtained by in situ photopolymn. of mixts. of a nonchiral diacrylate and a nonreactive compound with an antiferroelec. SmC*A phase-is described. Along with kinetic aspects from their photopolymn. processes, information has been obtained concerning the dielec. permittivity, spontaneous polarization, optical response to an applied elec. field, and the influence that the photopolymn. conditions and the structural characteristics of the network have on these properties. We have found that the polymer network not only stabilizes the antiferroelec. orientation but also alters the electro-optic properties of the liquid crystal.

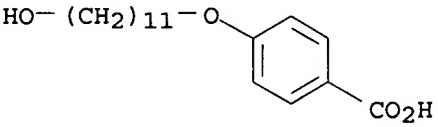
IT 1486-51-7, 4-Benzyloxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(chiral compound synthesis; synthesis and characterization of antiferroelec. liquid-crystal gels)

RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)

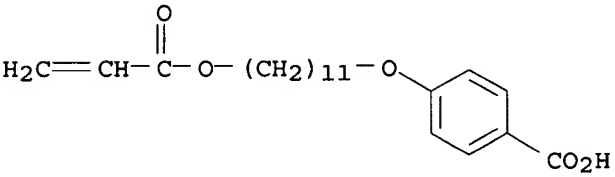


IT 59100-59-3P, 4-(11'-Hydroxyundecyloxy)benzoic acid
106620-90-0P, 4-(11'-Acryloyloxyundecyloxy)benzoic acid
351427-35-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crosslinker synthesis; synthesis and characterization of antiferroelec. liquid-crystal gels)

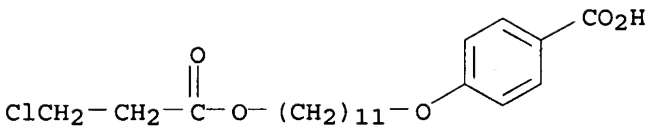
RN 59100-59-3 CAPLUS
CN Benzoic acid, 4-[(11-hydroxyundecyl)oxy]- (CA INDEX NAME)



RN 106620-90-0 CAPLUS
CN Benzoic acid, 4-[[11-[(1-oxo-2-propen-1-yl)oxy]undecyl]oxy]- (CA INDEX NAME)



RN 351427-35-5 CAPLUS
CN Benzoic acid, 4-[[11-(3-chloro-1-oxopropoxy)undecyl]oxy]- (9CI) (CA INDEX NAME)



RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 41 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:881140 CAPLUS
DN 134:42067
TI Indolylpiperidine derivatives, a method for their preparation and their use as antihistaminic and antiallergic agents
IN Pages Santacana, Lluis; Fonquerna Pou, Silvia; Puig Duran, Carles; Fernandez Forner, Dolors
PA Almirall Prodesfarma, S.A., Spain
SO PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000075130	A1	20001214	WO 2000-EP5010	20000531
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	ES 2165274	B1	20030401		
	CA 2375985	A1	20001214	CA 2000-2375985	20000531
	BR 2000011340	A	20020305	BR 2000-11340	20000531
	EP 1183251	A1	20020306	EP 2000-940296	20000531
	EP 1183251	B1	20040211		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, PT, IE, SI, LT, LV, FI, RO				
	TR 200103490	T2	20020422	TR 2001-3490	20000531
	JP 2003501424	T	20030114	JP 2001-502413	20000531
	EE 200100653	A	20030217	EE 2001-653	20000531
	EE 4717	B1	20061016		
	HU 200203320	A2	20030228	HU 2002-3320	20000531
	NZ 515649	A	20030829	NZ 2000-515649	20000531
	AT 259362	T	20040215	AT 2000-940296	20000531
	AU 773164	B2	20040520	AU 2000-55276	20000531
	PT 1183251	T	20040531	PT 2000-940296	20000531
	ES 2211559	T3	20040716	ES 2000-940296	20000531
	RU 2246493	C2	20050220	RU 2002-100073	20000531
	TW 226889	B	20050121	TW 2000-89110816	20000602
	IN 2001DN01075	A	20050311	IN 2001-DN1075	20011121
	ZA 2001009676	A	20030224	ZA 2001-9676	20011123
	NO 2001005897	A	20011203	NO 2001-5897	20011203
	MX 2001PA12425	A	20020604	MX 2001-PA12425	20011203
	BG 106168	A	20020731	BG 2001-106168	20011203
	US 2002147344	A1	20021010	US 2001-6416	20011204
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PRAI	ES 1999-1232	A	19990604		
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OS MARPAT 134:42067
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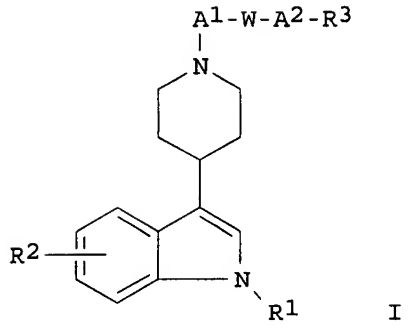


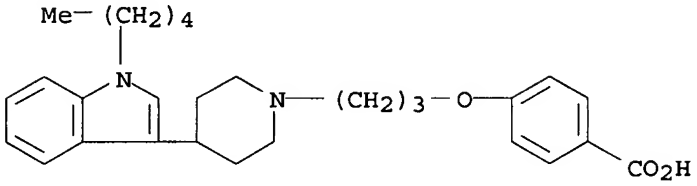
I

AB Indolylpiperidine compds. (I; A1 = alkylene, alkyleneoxy, alkylenethio, alkanoyl, hydroxyalkylene group; A2 = single bond, or alkylene or alkenylene group; W = single bond or phenylene or furanylene group which is unsubstituted or substituted by one or more halogen atoms, alkoxy groups and/or alkyl groups; R2 = H, halogen, alkyl, alkoxy group; and R3 = carboxyl or tetrazolyl group) are claimed. The present invention provides novel indolylpiperidine compds. and pharmaceutical compns. containing them having improved antihistamine and antiallergic activity with reduced cardiovascular or central nervous system side effects. Results of (1) histamine-H1 receptor binding assay, (2) histamine-induced skin vascular permeability in rats with the monitoring of antiallergic activity, (3) H1 ex-vivo binding studies in mice with the monitoring of degree of penetration into brain and (4) measurement of blood pressure and heart rate in conscious unrestrained hypertensive rats with the monitoring of cardiovascular effects, are presented. Processes for preparing the compds. are also claimed: (i) I (R3 = CO2R4; R4 = C1-4 alkyl) are hydrolyzed; (ii) I (R3 = CN) are reacted with an azide.

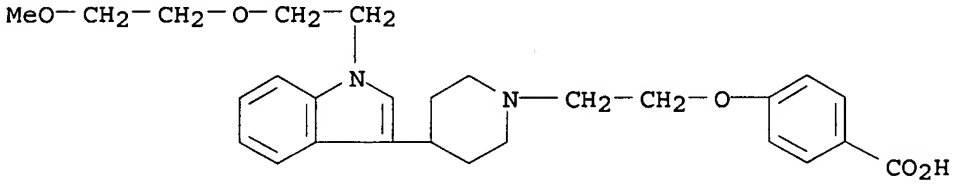
IT 312629-46-2P, 4-{3-[4-(1-Pentyl-1H-indol-3-yl)piperidin-1-yl]propoxy}benzoic acid 312629-52-0P, 4-[2-(4-{1-[2-(2-Methoxyethoxy)ethyl]-1H-indol-3-yl}piperidin-1-yl)ethoxy]benzoic acid 312629-53-1P, 4-{2-[4-(1-Pentyl-1H-indol-3-yl)piperidin-1-yl]ethoxy}benzoic acid 312629-61-1P, 4-[3-(4-{1-[2-(2-Methoxyethoxy)ethyl]-1H-indol-3-yl}piperidin-1-yl)propoxy]benzoic acid 312629-62-2P, 4-(3-{4-[1-(2-Ethoxyethyl)-1H-indol-3-yl]piperidin-1-yl}propoxy)benzoic acid 312630-37-8P, 2-(2-{4-[1-(2-Ethoxyethyl)-5-methoxy-1H-indol-3-yl]piperidin-1-yl}ethoxy)-4-methoxybenzoic acid 312630-38-9P, 2-(2-{4-[1-(2-Ethoxyethyl)-6-fluoro-1H-indol-3-yl]piperidin-1-yl}ethoxy)-4-methoxybenzoic acid 312630-39-0P, 2-(2-{4-[5-Bromo-1-(2-ethoxyethyl)-1H-indol-3-yl]piperidin-1-yl}ethoxy)-4-methoxybenzoic acid 312630-40-3P, 2-(2-{4-[7-Bromo-1-(2-ethoxyethyl)-1H-indol-3-yl]piperidin-1-yl}ethoxy)-4-methoxybenzoic acid 312630-41-4P, 2-(2-{4-[5-Chloro-1-(2-ethoxyethyl)-1H-indol-3-yl]piperidin-1-yl}ethoxy)-4-methoxybenzoic acid 312630-53-8P, 2-(2-{4-[1-(2-Ethoxyethyl)-4-fluoro-1H-indol-3-yl]piperidin-1-yl}ethoxy)-4-methoxybenzoic acid 312630-56-1P, 2-(2-{4-[4-Fluoro-1-(2-methoxyethyl)-1H-indol-3-yl]piperidin-1-yl}ethoxy)-4-methoxybenzoic acid 312630-86-7P, 2-(2-{4-[1-(2-Ethoxyethyl)-5-fluoro-1H-indol-3-yl]piperidin-1-yl}ethoxy)-4-methoxybenzoic acid 312630-92-5P, 4-(2-{4-[1-(2-Ethoxyethyl)-1H-indol-3-yl]piperidin-1-yl}ethoxy)benzoic acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(indolylpiperidine derivs., method for preparation and use as antihistaminic and antiallergic agents)

RN 312629-46-2 CAPLUS

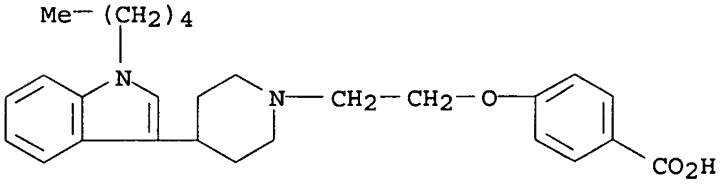
CN Benzoic acid, 4-[3-[4-(1-pentyl-1H-indol-3-yl)-1-piperidinyl]propoxy]- (9CI) (CA INDEX NAME)



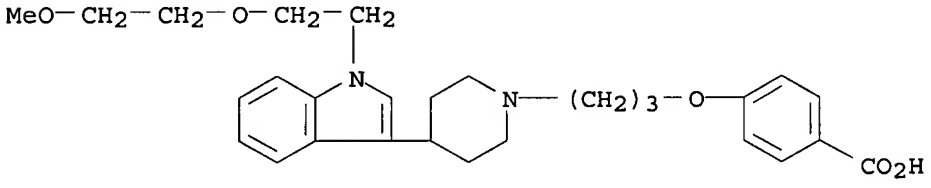
RN 312629-52-0 CAPLUS
CN Benzoic acid, 4-[2-[4-[1-[2-(2-methoxyethoxy)ethyl]-1H-indol-3-yl]-1-piperidinyl]ethoxy]- (9CI) (CA INDEX NAME)



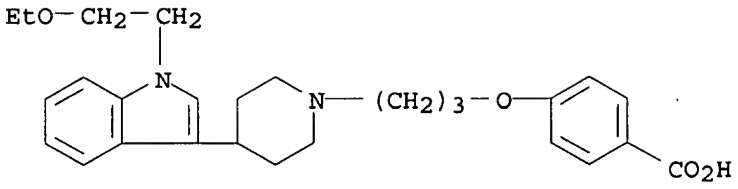
RN 312629-53-1 CAPLUS
CN Benzoic acid, 4-[2-[4-(1-pentyl-1H-indol-3-yl)-1-piperidinyl]ethoxy]- (9CI) (CA INDEX NAME)



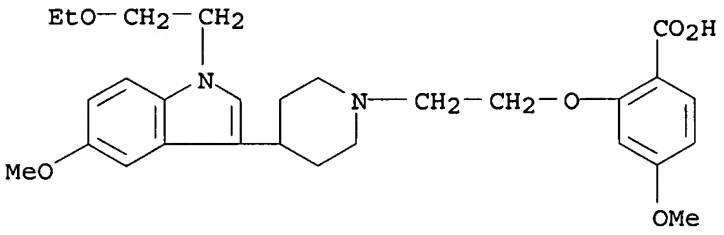
RN 312629-61-1 CAPLUS
CN Benzoic acid, 4-[3-[4-[1-[2-(2-methoxyethoxy)ethyl]-1H-indol-3-yl]-1-piperidinyl]propoxy]- (9CI) (CA INDEX NAME)



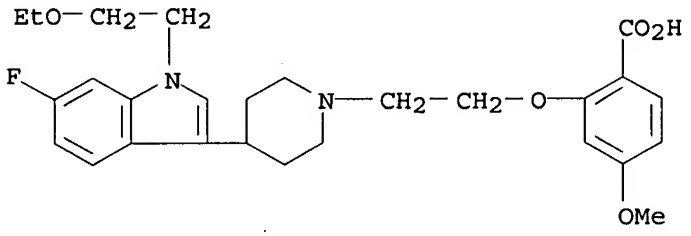
RN 312629-62-2 CAPLUS
CN Benzoic acid, 4-[3-[4-[1-(2-ethoxyethyl)-1H-indol-3-yl]-1-piperidinyl]propoxy]- (9CI) (CA INDEX NAME)



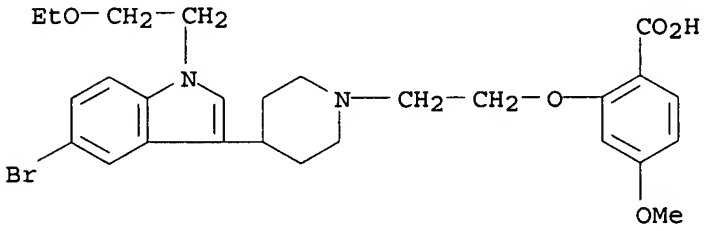
RN 312630-37-8 CAPLUS
CN Benzoic acid, 2-[2-[4-[1-(2-ethoxyethyl)-5-methoxy-1H-indol-3-yl]-1-piperidinyl]ethoxy]-4-methoxy- (9CI) (CA INDEX NAME)



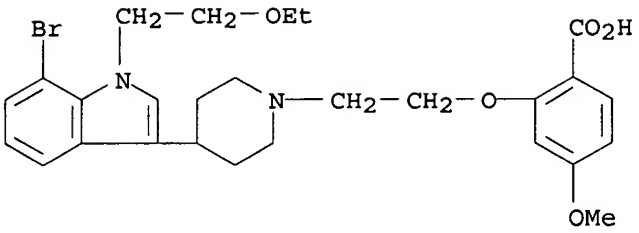
RN 312630-38-9 CAPLUS
CN Benzoic acid, 2-[2-[4-[1-(2-ethoxyethyl)-6-fluoro-1H-indol-3-yl]-1-piperidinyl]ethoxy]-4-methoxy- (9CI) (CA INDEX NAME)



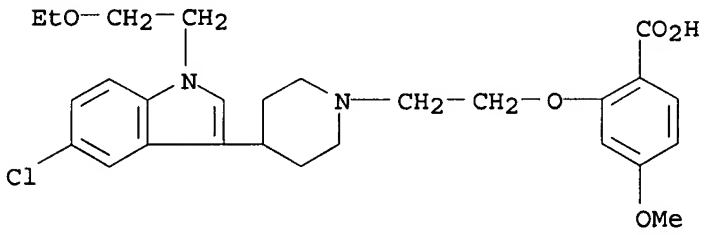
RN 312630-39-0 CAPLUS
CN Benzoic acid, 2-[2-[4-[5-bromo-1-(2-ethoxyethyl)-1H-indol-3-yl]-1-piperidinyl]ethoxy]-4-methoxy- (9CI) (CA INDEX NAME)



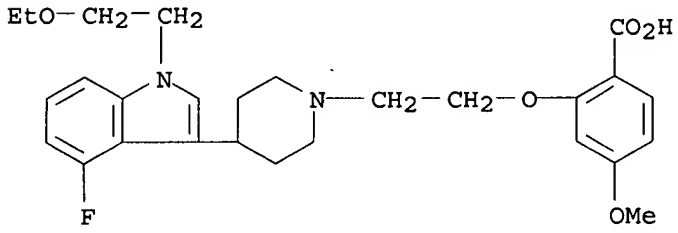
RN 312630-40-3 CAPLUS
CN Benzoic acid, 2-[2-[4-[7-bromo-1-(2-ethoxyethyl)-1H-indol-3-yl]-1-piperidinyl]ethoxy]-4-methoxy- (9CI) (CA INDEX NAME)



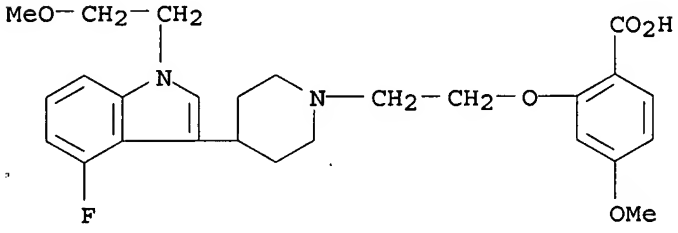
RN 312630-41-4 CAPLUS
CN Benzoic acid, 2-[2-[4-[5-chloro-1-(2-ethoxyethyl)-1H-indol-3-yl]-1-piperidinyl]ethoxy]-4-methoxy- (9CI) (CA INDEX NAME)



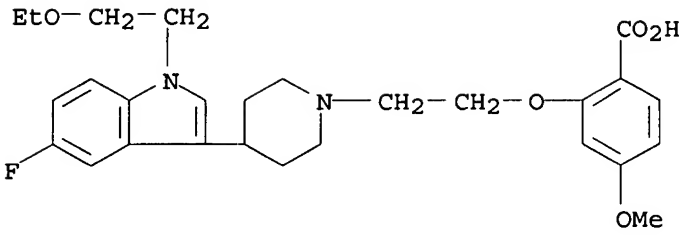
RN 312630-53-8 CAPLUS
CN Benzoic acid, 2-[2-[4-[1-(2-ethoxyethyl)-4-fluoro-1H-indol-3-yl]-1-piperidinyl]ethoxy]-4-methoxy- (9CI) (CA INDEX NAME)



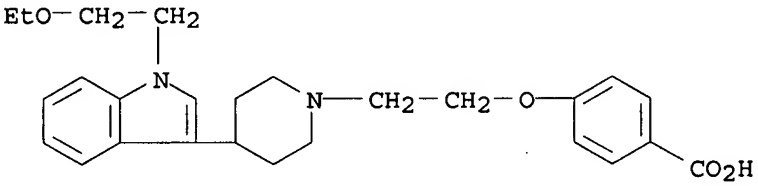
RN 312630-56-1 CAPLUS
CN Benzoic acid, 2-[2-[4-[4-fluoro-1-(2-methoxyethyl)-1H-indol-3-yl]-1-piperidinyl]ethoxy]-4-methoxy- (9CI) (CA INDEX NAME)



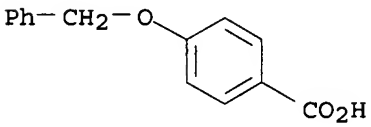
RN 312630-86-7 CAPLUS
CN Benzoic acid, 2-[2-[4-[1-(2-ethoxyethyl)-5-fluoro-1H-indol-3-yl]-1-piperidinyl]ethoxy]-4-methoxy- (9CI) (CA INDEX NAME)



RN 312630-92-5 CAPLUS
CN Benzoic acid, 4-[2-[4-[1-(2-ethoxyethyl)-1H-indol-3-yl]-1-piperidinyl]ethoxy]- (9CI) (CA INDEX NAME)



IT 1486-51-7P, 4-Benzyloxybenzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate in preparation of indolylpiperidine derivs.)
RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 42 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:742063 CAPLUS
DN 133:309794
TI methods for their preparation of catechin and epicatechin dimers
IN Tuckmantel, Werner; Kozikowski, Alan P.; Romanczyk, Leo J.
PA Mars, Incorporated, USA
SO PCT Int. Appl., 22 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

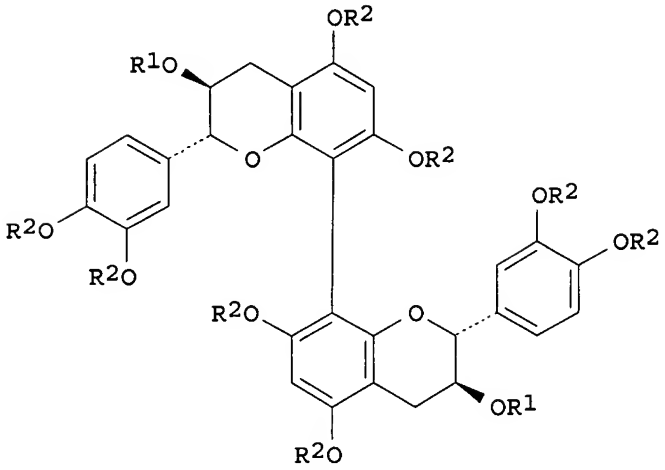
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000061547	A1	20001019	WO 2000-US8234	20000329

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

	US 6156912	A	20001205	US 1999-289565	19990409
	CA 2369399	A1	20001019	CA 2000-2369399	20000329
	EP 1169304	A1	20020109	EP 2000-919756	20000329
	EP 1169304	B1	20040929		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2002541241	T	20021203	JP 2000-610824	20000329
	AT 277899	T	20041015	AT 2000-919756	20000329
	ES 2230089	T3	20050501	ES 2000-919756	20000329
	AU 782592	B2	20050811	AU 2000-40389	20000329
	IL 145788	A	20051120	IL 2000-145788	20000329
	RU 2293081	C2	20070210	RU 2001-130139	20000329
PRAI	US 1999-289565	A	19990409		
	WO 2000-US8234	W	20000329		

OS CASREACT 133:309794

GI



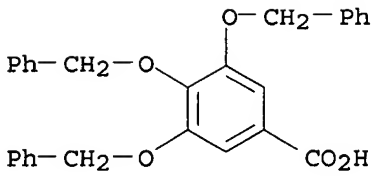
I

AB A process for preparing catechin and epicatechin dimers with (8-8), (6-6), and (8-6) linkages as well as digalloyl dimers is disclosed which involves the oxidative or reductive coupling of protected monomers. Thus, preparation of 3,3"-di-O-galloyl-8,8"-bicatechin (I: R1 = galloyl, R2 = H) (II) comprises the steps of: (a) protecting phenolic and alc. hydroxyl groups with benzyl and tetrahydropyranyl groups resp.; (b) halogenating the compds. of step (a) to introduce a halo group at the C-8 position; (c) reacting the compds. of step (b) with an aryl lithium compound to introduce lithium at C-8 positions; (d) oxidatively or reductively coupling of compds. of step (c) followed by deprotection of the 3-hydroxyl positions; (e) esterifying the compound of step (d) with tri-O-benzylgalloyl halide to form protected digalloyl ester I (R1 = tri-O-benzylgalloyl, R2 = CH2Ph) which on deprotection affords II.

IT 1486-48-2, Tri-O-benzylgallic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of catechin and epicatechin dimers)

RN 1486-48-2 CAPLUS

CN Benzoic acid, 3,4,5-tris(phenylmethoxy)- (CA INDEX NAME)

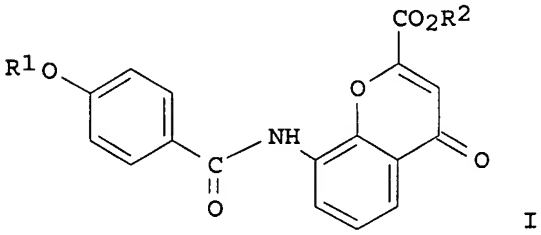


RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

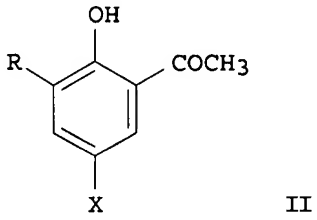
L15 ANSWER 43 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:78497 CAPLUS
DN 130:153574
TI Preparation of (benzoylamino)benzopyrancarboxylates and their intermediates
IN Tsunemine, Masami; Akagi, Miyoko; Muto, Nobuo; Kishimoto, Shuichi; Shiramizu, Masanao; Akasaki, Shizuo; Otoku, Yoshimi; Kodera, Kaoru
PA Showa Chemical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11029540	A	19990202	JP 1997-195168	19970704

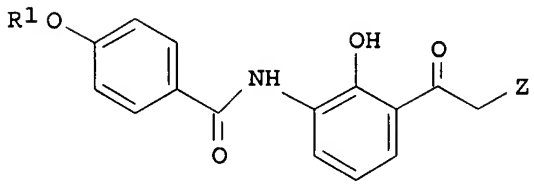
PRAI JP 1997-195168 19970704
OS CASREACT 130:153574; MARPAT 130:153574
GI



I



II



III

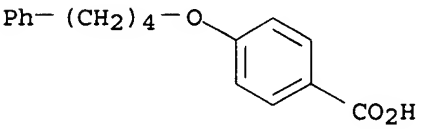
AB Title compds. I [R1 = (Ph-substituted) C2-5 alkyl; R2 = C1-4 alkyl], useful as intermediates for pharmaceuticals and agrochems., are prepared by catalytic reduction of acetophenones II (R = NO2; X = halo) in aromatic hydrocarbon solvents, pH adjustment with bases, catalytic reductive dehalogenation of II (R = NH2; X = halo), amidation of II (R = NH2; X = H) with p-R1OC6H4COY (R1 = same as I; Y = halo) in the presence of MmBn (M = alkali metal, alkaline earth metal; B = lower fatty acid anion, phosphate-type anion; m, n > 0), reaction of amides III (R1 = same as I; Z = H) with (CO2R2)2 (R2 = same as I) and alcoholates, and treatment of III (Z = COCO2R2) with acids. The process can be carried out without

isolation of intermediates. A PhMe solution of III [R1 = (CH2)4Ph, Z = H] (preparation given) was treated with (CO2Me)2 and MeONa at 70° for 1 h and treated with MeSO3H at 75° for 3 h to give 77.9% I [R1 = (CH2)4Ph, R2 = Me], which can be converted into pranlukast.

IT 30131-16-9, 4-(4-Phenylbutoxy)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (benzoylamino)benzopyrancarboxylates as intermediate for pranlukast)

RN 30131-16-9 CAPLUS

CN Benzoic acid, 4-(4-phenylbutoxy)- (CA INDEX NAME)



L15 ANSWER 44 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1997:502263 CAPLUS

DN 127:121498

TI Method for producing optically active and inactive 1-hydroxy-2,2,2-trifluoroethyl ω-ethoxyalkyl ketones as intermediates for ferroelectric liquid crystals

IN Kubota, Toshio; Iijima, Norihisa

PA Toa Gosei Chemical Industry Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 53 pp.
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 09176077	A	19970708	JP 1995-350073	19951225
PRAI JP 1995-350073		19951225		

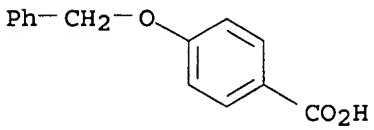
OS CASREACT 127:121498; MARPAT 127:121498

AB Racemic CF3CH(OH)CO(CH2)mOEt (I) (m = 3-6) is prepared by addition reaction of 2-hydroxy-3,3,3-trifluoropropionitrile with EtO(CH2)mMgBr in an organic solvent followed by hydrolysis with mineral acid. Optically active (S)- and (R)-I are prepared by esterification of racemic I with (S)-2-acetoxypropionyl chloride (resolving agent) and silica gel chromatog. separation of the resulting diastereomer mixture followed by hydrolysis with mineral acid. I is useful as intermediates for antiferroelec. liquid crystal compds. or also as building blocks, to which various functional groups can be introduced, for drugs and agrochems. This process efficiently gives I in high yields and above optical resolution process provides an industrial optical resolution with long-term operational stability and high resolution ratio. Thus, a solution of 153.3 g 4-ethoxybutylmagnesium bromide (preparation given) in Et2O was added dropwise to 42.5 g 2-hydroxy-3,3,3-trifluoropropionitrile in Et2O at 0° over 110 min in an ice-bath, stirred for 2 h, warmed to room temperature, treated dropwise with 340 mL 3.5 N HCl over 34 min, and stirred for 20 min to give 80% racemic 1-hydroxy-2,2,2-trifluoroethyl 4-ethoxybutyl ketone. The latter racemate (60.4 g) and 43.9 g (S)-2-acetoxypropionyl chloride were placed in a flask and heated with stirring in vacuo at 180 mmHg and 50° under reflux for 31 min and then at 50 mmHg and 95° under reflux for 47 min to give a 1:1 diastereomer mixture of (2S)- and (2R)-2-[(2S)-2-acetoxypropionyloxy]-7-ethoxy-1,1,1-trifluoroheptan-3-one (90%). This mixture was separated by medium pressure liquid chromatog. using a LOBAR column RECHROPREP. Si60 and eluting the column

with n-hexane/CHCl3 (80/20) to give 45% (2S)-2-[(2S)-2-acetoxypropionyloxy]-7-ethoxy-1,1,1-trifluoroheptan-3-one and 45% (2R)-2-[(2S)-2-acetoxypropionyloxy]-7-ethoxy-1,1,1-trifluoroheptan-3-one, each of which was refluxed in a mixture of 3.5 N HCl and MeOH at 80° for 2 h to give 90% (S)-1-hydroxy-2,2,2-trifluoroethyl 4-ethoxybutyl ketone and 90% (R)-1-hydroxy-2,2,2-trifluoroethyl 4-ethoxybutyl ketone.

IT 1486-51-7, 4-Benzyloxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of optically active 1-hydroxy-2,2,2-trifluoroethyl ω-ethoxyalkyl ketones and their derivs. by resolution using (S)-2-acetoxypropionyl chloride)

RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



L15 ANSWER 45 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1997:502262 CAPLUS
DN 127:121497
TI Method for producing optically active anti- and syn-2-hydroxy-3-methoxy-ω-ethoxyalkane as intermediates for ferroelectric liquid crystals
IN Kubota, Toshio; Iijima, Norihisa
PA Toa Gosei Chemical Industry Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 55 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 09176072	A	19970708	JP 1995-350059	19951225
PRAI	JP 1995-350059		19951225		

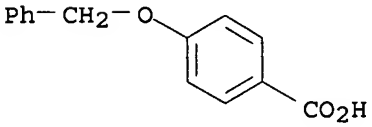
OS CASREACT 127:121497; MARPAT 127:121497
AB Anti-(2S,3S)- and syn-(2S,3R)-CF3CH(OH)CH(OMe)(CH2)mOEt (I) (m = 3-6) or anti-(2R,3R)- and syn-(2R,3S)-I are prepared by reduction of (S)- or (R)-1-hydroxy-2,2,2-trifluoroethyl ω-ethoxyalkyl ketone, i.e. (S)- or (R)-CF3CH(OH)CO(CH2)mOEt, resp., with a metal hydride, reaction of the resulting diols with a alkali metal hydride and then with AcCl, reaction of the resulting O-acetylated derivs. with MeI , alkali hydrolysis of the resulting O-methylated derivs., and separation of the resulting diastereomers. This process efficiently gives in high yields I which are useful as intermediates for antiferroelec. liquid crystal compds. or also as building blocks, to which various functional groups can be introduced, for drugs and agrochems. (S)-1-hydroxy-2,2,2-trifluoroethyl 4-ethoxybutyl ketone (preparation given) was reduced by LiAlH4 in Et2O at room temperature for 6 h to give a diastereomeric mixture of anti-(2S,3S)- and syn-(2S,3R)-7-ethoxy-1,1,1-trifluoroheptane-2,3-diol in 95% yield. This mixture in Et2O was added dropwise to a mixture of NaH in Et2O under ice-cooling and stirred at room temperature for 60 min followed by adding dropwise AcCl in Et2O at 0° and the resulting mixture was stirred for 120 min to give a diastereomeric mixture of anti-(2S,3S)- and syn-(2S,3R)-2-acetoxy-7-ethoxy-1,1,1-trifluoroheptan-3-ol. This alc. mixture was similarly treated with NaH followed by adding dropwise MeI in Et2O at 0° and the resulting mixture was stirred for 120 min to give a diastereomeric mixture of anti-(2S,3S)- and syn-(2S,3R)-2-acetoxy-7-ethoxy--3-methoxy-1,1,1-trifluoroheptane. This mixture was stirred with K2CO3 in MeOH at room temperature

for 3 h to give a 88/12 diastereomeric mixture of anti-(2S,3S)- and syn-(2S,3R)-I, which was separated by medium pressure liquid chromatog. using a LOBAR column RECHROPREP. Si60 an eluting the column with n-hexane/isopropanol (95/5 volume ratio) to give 10.8% anti-(2S,3S)-I and 79.2% syn-(2S,3R)-I.

IT 1486-51-7, 4-Benzyloxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of optically active anti- and syn-2-hydroxy-3-methoxy-ω-ethoxyalkane via reduction of hydroxytrifluoroethyl ω-ethoxyalkyl ketone)

RN 1486-51-7 CAPLUS

CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



L15 ANSWER 46 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1997:328796 CAPLUS

DN 126:305466

TI Preparation of 3-[[4-(4-phenylbutoxy)benzoyl]amino]-2-hydroxyacetophenone as a drug intermediate

IN Fukuda, Etsuko; Furutani, Atsushi; Ushio, Hideki; Murata, Hirokazu

PA Sumitomo Chemical Company Limited, Japan

SO Brit. UK Pat. Appl., 26 pp.
CODEN: BAXXDU

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 2302873	A	19970205	GB 1996-13610	19960628
	GB 2302873	B	19980923		
	JP 09071558	A	19970318	JP 1996-164379	19960625
	JP 3487081	B2	20040113		
	US 5675036	A	19971007	US 1996-673441	19960628
PRAI	JP 1995-163551	A	19950629		

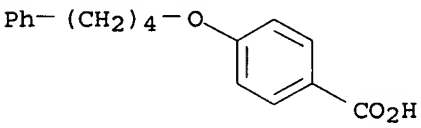
OS CASREACT 126:305466; MARPAT 126:305466

AB The title process comprises etherification of 4-(HO)C6H4CO2R (R = alkyl) by Ph(CH2)4X (X = halo) in the presence of a base, an aprotic polar compound, and a hydrocarbon solvent followed by the steps of saponification, acid halide formation, and amidation of 3-amino-2-hydroxyacetophenone.

IT 30131-16-9P, 4-(4-Phenylbutoxy)benzoic acid
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-[[4-(4-phenylbutoxy)benzoyl]amino]-2-hydroxyacetophenone as a drug intermediate)

RN 30131-16-9 CAPLUS

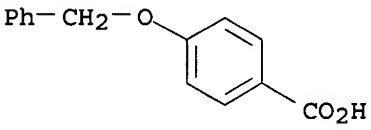
CN Benzoic acid, 4-(4-phenylbutoxy)- (CA INDEX NAME)



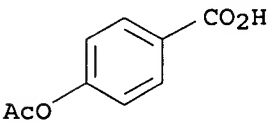
L15 ANSWER 47 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1997:324148 CAPLUS
DN 126:299708
TI Aminoalkyl 4-hydroxybenzoate derivative as an additive for heat-sensitive printing material
IN Nigorikawa, Kazunori
PA Fuji Photo Film Co Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 09067321	A	19970311	JP 1995-227736	19950905
JP 3725587	B2	20051214		
PRAI JP 1995-227736		19950905		

OS MARPAT 126:299708
AB 4-HOC6H4CO2CnH2nNR1R2 (R1, R2 = C4-6 linear or branched alkyl; n = 2-9; the benzene ring may be substituted with halo, OH, lower alkyl, lower alkoxy) are claimed. The 4-hydroxybenzoates are useful as accelerators for diazo coupling reaction or color fading for electron-donating leuco dye colors in heat-sensitive printing materials.
IT 1486-51-7, 4-Benzyloxybenzoic acid 2345-34-8, 4-Acetyloxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aminoalkyl 4-hydroxybenzoates as diazo coupling and color fading accelerators for heat-sensitive printing)
RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



RN 2345-34-8 CAPLUS
CN Benzoic acid, 4-(acetyloxy)- (CA INDEX NAME)



L15 ANSWER 48 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1997:320831 CAPLUS
DN 127:17491
TI Process for preparation of alkoxybenzoic acid derivatives
IN Otsuji, Atsuo; Ishida, Tsutomu; Totani, Yoshiyuki; Hirao, Motokazu; Kayashima, Hiroe; Nakatsuka, Masakatsu
PA Mitsui Toatsu Chemicals, Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 16 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

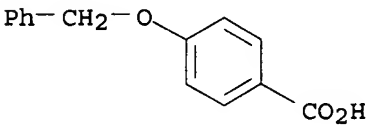
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 09077717	A	19970325	JP 1995-235200	19950913

PRAI JP 1995-235200 19950913

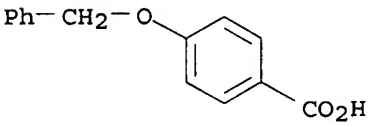
AB Claimed is a process for preparation of the title compds. (I) by (a) alkylation of hydroxybipnenylcarboxylic acid or ester derivs., (b) separation of the basic salt obtained, and (c) contacting with acids. I, useful as intermediates in the production of functional materials, drugs and pesticides, are prepared in an industrial manner efficiently and easily. Thus, HO-p-C6H4CO2H was reacted with Ph(CH2)4Br in the presence of KOH and then treated with aqueous HCl in H2O after separation of acid potassium salt to give the title compound Ph(CH2)4O-p-C6H4CO2H with 99.5% purity.

IT 56442-48-9P 56442-54-7P 65212-75-1P 147308-45-0P 189135-67-9P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for preparation of alkoxybenzoic acid derivs.)

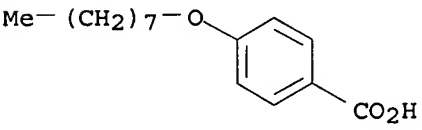
RN 56442-48-9 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)-, sodium salt (9CI) (CA INDEX NAME)



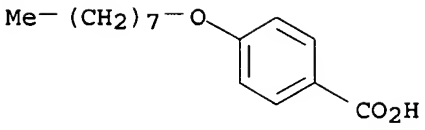
RN 56442-54-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)-, potassium salt (9CI) (CA INDEX NAME)



RN 65212-75-1 CAPLUS
CN Benzoic acid, 4-(octyloxy)-, sodium salt (1:1) (CA INDEX NAME)

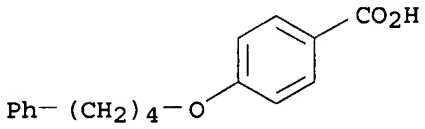


RN 147308-45-0 CAPLUS
CN Benzoic acid, 4-(octyloxy)-, potassium salt (9CI) (CA INDEX NAME)



● K

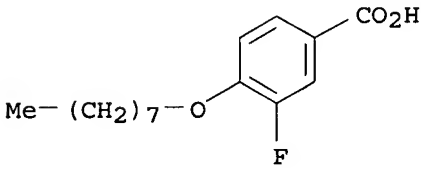
RN 189135-67-9 CAPLUS
CN Benzoic acid, 4-(4-phenylbutoxy)-, potassium salt (9CI) (CA INDEX NAME)



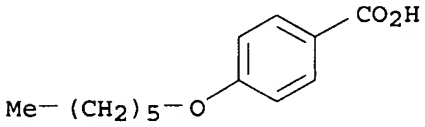
● K

IT 326-78-3P 1142-39-8P 1486-51-7P
1498-96-0P 2493-84-7P 5519-23-3P
15872-46-5P 30131-16-9P 95880-52-7P
112789-77-2P 122265-96-7P 124055-05-6P
127806-89-7P 128895-76-1P 189135-63-5P
189135-64-6P 189135-65-7P 189135-66-8P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for preparation of alkoxybenzoic acid derivs.)

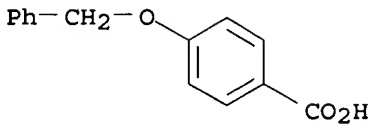
RN 326-78-3 CAPLUS
CN Benzoic acid, 3-fluoro-4-(octyloxy)- (9CI) (CA INDEX NAME)



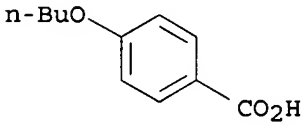
RN 1142-39-8 CAPLUS
CN Benzoic acid, 4-(hexyloxy)- (CA INDEX NAME)



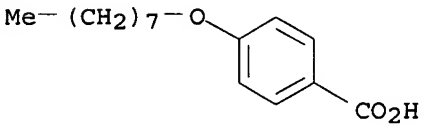
RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



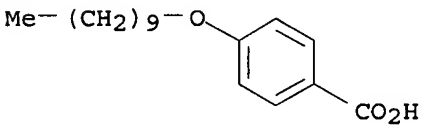
RN 1498-96-0 CAPLUS
CN Benzoic acid, 4-butoxy- (CA INDEX NAME)



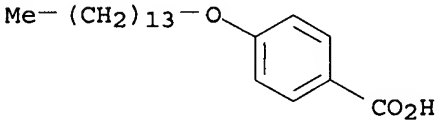
RN 2493-84-7 CAPLUS
CN Benzoic acid, 4-(octyloxy)- (CA INDEX NAME)



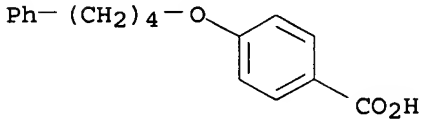
RN 5519-23-3 CAPLUS
CN Benzoic acid, 4-(decyloxy)- (CA INDEX NAME)



RN 15872-46-5 CAPLUS
CN Benzoic acid, 4-(tetradecyloxy)- (CA INDEX NAME)

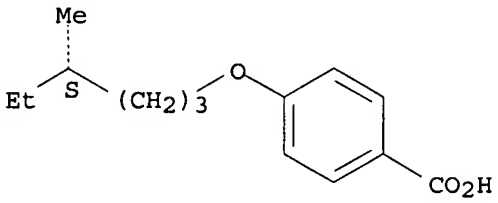


RN 30131-16-9 CAPLUS
CN Benzoic acid, 4-(4-phenylbutoxy)- (CA INDEX NAME)



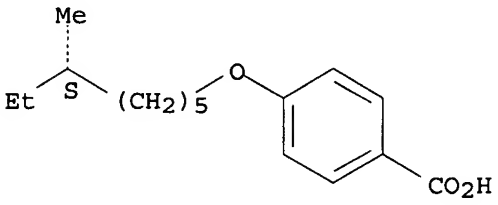
RN 95880-52-7 CAPLUS
CN Benzoic acid, 4-[[(4S)-4-methylhexyl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

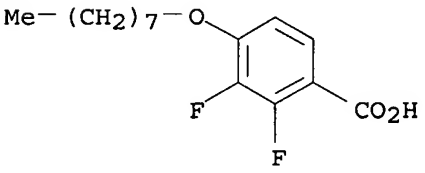


RN 112789-77-2 CAPLUS
CN Benzoic acid, 4-[(6-methyloctyl)oxy]-, (S)- (9CI) (CA INDEX NAME)

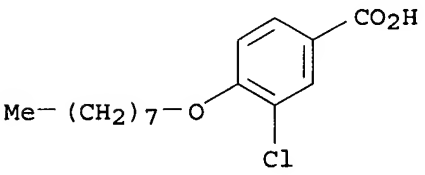
Absolute stereochemistry.



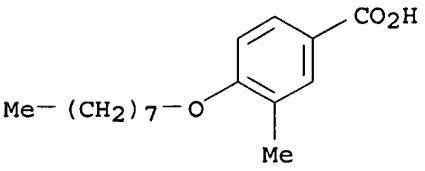
RN 122265-96-7 CAPLUS
CN Benzoic acid, 2,3-difluoro-4-(octyloxy)- (9CI) (CA INDEX NAME)



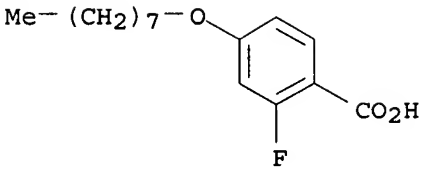
RN 124055-05-6 CAPLUS
CN Benzoic acid, 3-chloro-4-(octyloxy)- (9CI) (CA INDEX NAME)



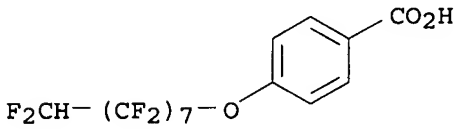
RN 127806-89-7 CAPLUS
CN Benzoic acid, 3-methyl-4-(octyloxy)- (9CI) (CA INDEX NAME)



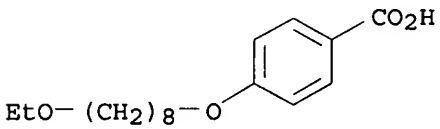
RN 128895-76-1 CAPLUS
CN Benzoic acid, 2-fluoro-4-(octyloxy)- (9CI) (CA INDEX NAME)



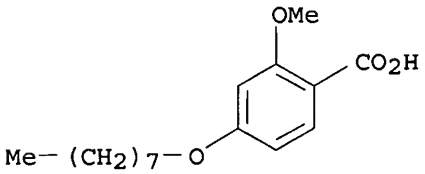
RN 189135-63-5 CAPLUS
CN Benzoic acid, 4-[(1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-hexadecafluorooctyl)oxy]- (9CI) (CA INDEX NAME)



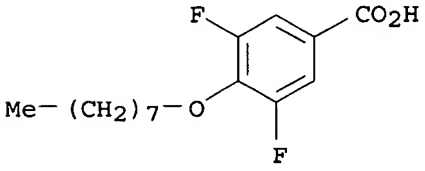
RN 189135-64-6 CAPLUS
CN Benzoic acid, 4-[(8-ethoxyoctyl)oxy]- (9CI) (CA INDEX NAME)



RN 189135-65-7 CAPLUS
CN Benzoic acid, 2-methoxy-4-(octyloxy)- (9CI) (CA INDEX NAME)

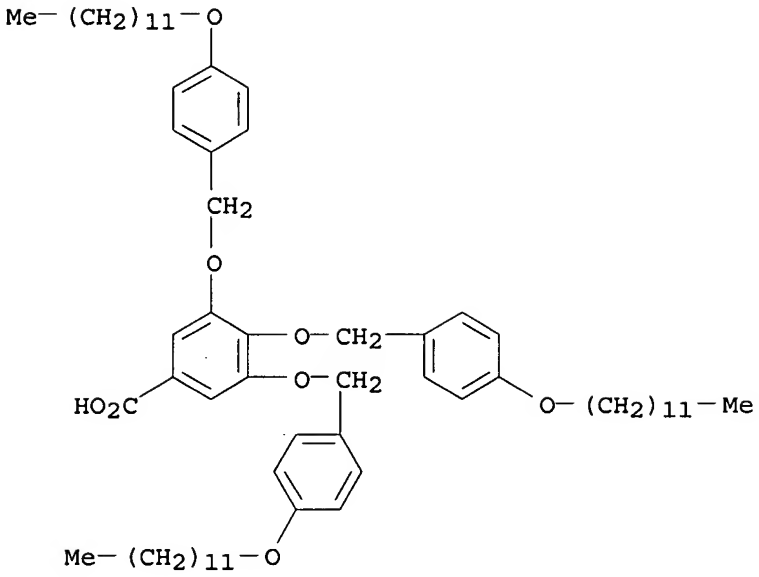


RN 189135-66-8 CAPLUS
CN Benzoic acid, 3,5-difluoro-4-(octyloxy)- (9CI) (CA INDEX NAME)

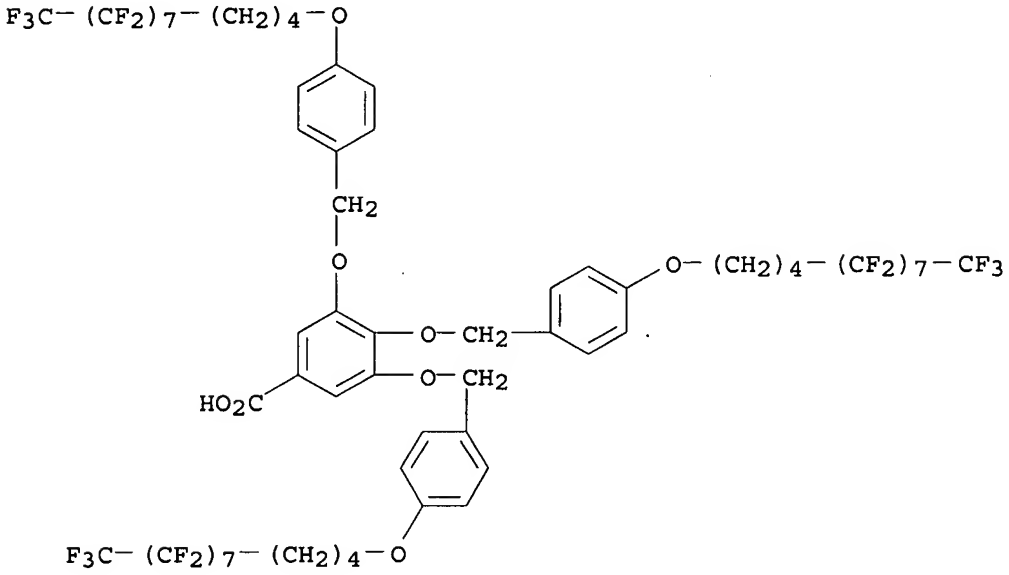


L15 ANSWER 49 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1996:616694 CAPLUS
DN 125:343496
TI Fluorophobic Effect Induces the Self-Assembly of Semifluorinated Tapered Monodendrons Containing Crown Ethers into Supramolecular Columnar Dendrimers Which Exhibit a Homeotropic Hexagonal Columnar Liquid Crystalline Phase
AU Percec, Virgil; Johansson, Gary; Ungar, Goran; Zhou, Jianping

CS Department of Macromolecular Science, Case Western Reserve University, Cleveland, OH, 44106-7202, USA
SO Journal of the American Chemical Society (1996), 118(41), 9855-9866
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB The rational design, synthesis, and characterization of the building blocks obtained by the esterification of the 1st generation of tapered monodendrons 3,4,5-tris(p-dodecan-1-yloxy)benzoic acid (12-AG) and 3,4,5-tris[p-(n-dodecan-1-yloxy)benzyloxy]benzoic acid (12-ABG) containing semifluorinated dodecyl groups [i.e., 12Fn-AG-15C5 (n = 0, 4, 6, 8), 12Fn-AG-B15C5, 12Fn-ABG-15C5, and 12Fn-ABG-B15C5 (n = 0 and 8) where n following the letter F represents the number of outer perfluorinated methylenic units of the dodecyl group] with 4'-hydroxymethyl(benzo-15-crown-5) (B15C5) and 1-hydroxymethyl(15-crown-5) (15C5) are described. All building blocks self-assemble into supramol. cylindrical or rod-like dendrimers via ion-mediated complexation processes. These rod-like supermols. form a thermotropic hexagonal columnar (Φh) liquid crystalline (LC) phase. The fluorination of the dodecyl groups of these tapered building blocks enhances dramatically their self-assembly ability. The building blocks based on n = 6 and 8 self-assemble into supramol. columns solely via the fluorophobic effect. Direct structural characterization of the supramol. columns obtained via these two mol. recognition processes by a combination of techniques consisting of DSC, x-ray diffraction, and thermal optical polarized microscopy, and of the columns obtained solely via the fluorophobic effect allowed the construction of mol. models for the supramol. columns obtained via these two organizing forces. An increase in the column diameter with increasing n and with the complexation of metal salts (i.e., alkali metal trifluoromethanesulfonates) accounts for a structural model in which the uncomplexed and complexed crown ethers are placed side-by-side in the center of the column with the melted tapered side groups radiating toward its periphery. The perfluorinated segments of the building blocks are microsegregated from the perhydrogenated and aromatic segments of the column. The supramol. columns obtained from building blocks with n = 8 align homeotropically in the Φh LC phase on untreated glass slides, i.e., form single crystal liquid crystals in which the long axes of their columns are perpendicular to the glass surface. Both the self-assembly of supramol. columns induced solely by the fluorophobic effect and the homeotropic alignment of these columns in their Φh LC phase open extremely interesting new synthetic and technol. opportunities in the area of self-assembly of well-defined supramol. architectures obtained from monodendrons and other building blocks.
IT 110934-58-2P 183578-50-9P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and liquid crystal properties and fluorophobic effect on self-assembly of)
RN 110934-58-2 CAPLUS
CN Benzoic acid, 3,4,5-tris[[4-(dodecyloxy)phenyl]methoxy]- (CA INDEX NAME)



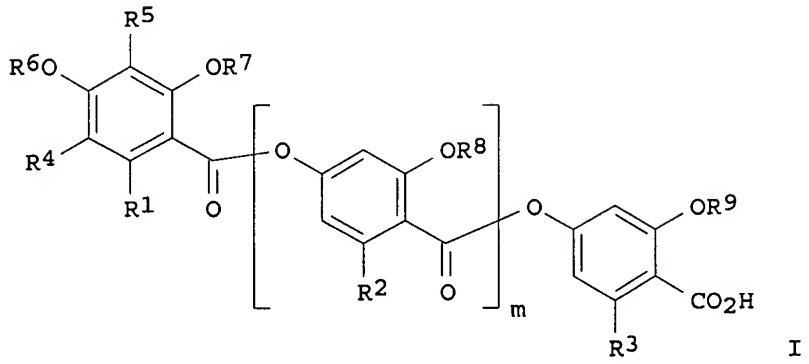
RN 183578-50-9 CAPLUS
CN Benzoic acid, 3,4,5-tris[[4-[(5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heptadecafluorododecyl)oxy]phenyl]methoxy]- (CA INDEX NAME)



L15 ANSWER 50 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1996:593967 CAPLUS
DN 125:212679
TI Phosphodiesterase inhibitor and process for producing the same
IN Ishida, Koichi; Enomoto, Mitsuo; Fujita, Shinji; Oka, Hiroko
PA Nippon Kayaku Kabushiki Kaisha, Japan
SO PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9625386	A1	19960822	WO 1996-JP316	19960214

W: CA, CN, KR, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
JP 08283149 A 19961029 JP 1996-49637 19960214
PRAI JP 1995-49304 A 19950215
OS MARPAT 125:212679
GI

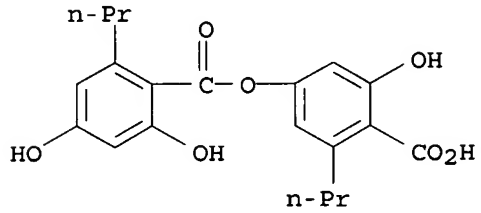


I

AB A phosphodiesterase inhibitor comprises as the active ingredient 6-substituted-β-resorcylic acid derivs. represented by general formula (I) or pharmacol. acceptable salts thereof: wherein m represents 0 or 1; R1, R2 and R3 represent each lower alkyl; R4 and R5 represent each hydrogen or halogeno; and R6, R7, R8 and R9 represent each hydrogen or lower alkyl. The phosphodiesterase inhibitor is expected to be applicable to, for example, remedies for bronchial asthma, bronchitis, allergic diseases, cardiac circulatory diseases, brain diseases, immune diseases, inflammatory diseases, etc. As an example, compds. NF00634-1, NF00634-2, NF00634-3, NF00634-4 and NF00634-5 were manufactured by incubation of Dendrodochium NF-00634 in a medium containing soluble starch, glucose, corn steep liquor, Pronal ST-1, and salts at 25° for 3 days and chromatog. purification Organic syntheses of NF00634-1 (PD-001) and related compds. also are presented.

IT 64756-85-0P
RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(therapeutic phosphodiesterase inhibitor and process for producing the same)

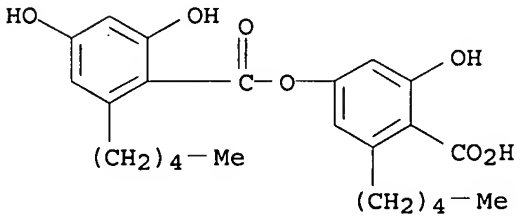
RN 64756-85-0 CAPLUS
CN Benzoic acid, 2,4-dihydroxy-6-propyl-, 4-carboxy-3-hydroxy-5-propylphenyl ester (9CI) (CA INDEX NAME)



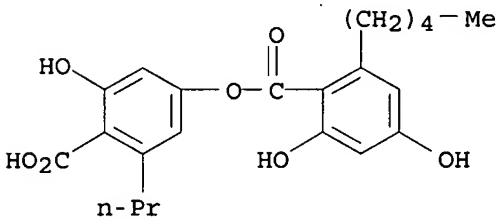
IT 641-68-9P 67121-42-0P
RL: BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL

(Biological study); PREP (Preparation); USES (Uses)
(therapeutic phosphodiesterase inhibitor and process for producing the same)

RN 641-68-9 CAPLUS
CN Benzoic acid, 2,4-dihydroxy-6-pentyl-, 4-carboxy-3-hydroxy-5-pentylphenyl ester (9CI) (CA INDEX NAME)

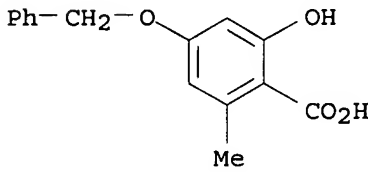


RN 67121-42-0 CAPLUS
CN Benzoic acid, 2,4-dihydroxy-6-pentyl-, 4-carboxy-3-hydroxy-5-propylphenyl ester (9CI) (CA INDEX NAME)

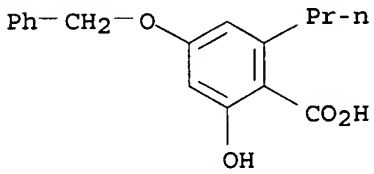


IT 54102-37-3P 104307-64-4P 181577-45-7P
181577-56-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(therapeutic phosphodiesterase inhibitor and process for producing the same)

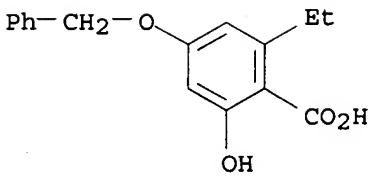
RN 54102-37-3 CAPLUS
CN Benzoic acid, 2-hydroxy-6-methyl-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



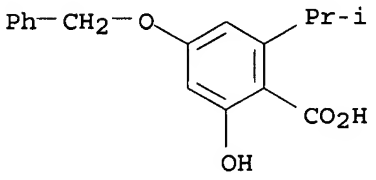
RN 104307-64-4 CAPLUS
CN Benzoic acid, 2-hydroxy-4-(phenylmethoxy)-6-propyl- (9CI) (CA INDEX NAME)



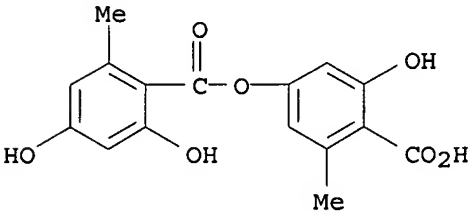
RN 181577-45-7 CAPLUS
CN Benzoic acid, 2-ethyl-6-hydroxy-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



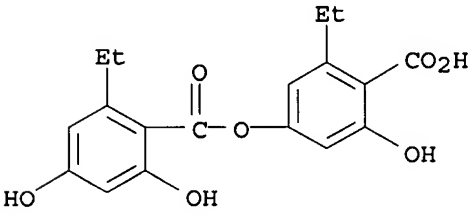
RN 181577-56-0 CAPLUS
CN Benzoic acid, 2-hydroxy-6-(1-methylethyl)-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



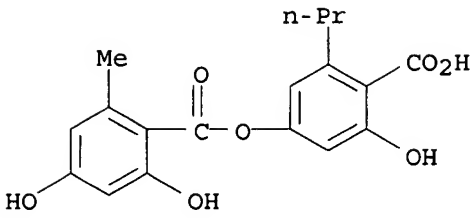
IT 480-56-8P 181577-36-6P 181577-38-8P
181577-39-9P 181577-41-3P 181577-42-4P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(therapeutic phosphodiesterase inhibitor and process for producing the same)
RN 480-56-8 CAPLUS
CN Benzoic acid, 2,4-dihydroxy-6-methyl-, 4-carboxy-3-hydroxy-5-methylphenyl ester (CA INDEX NAME)



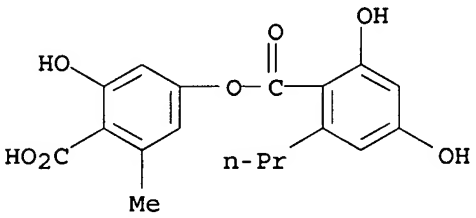
RN 181577-36-6 CAPLUS
CN Benzoic acid, 2-ethyl-4,6-dihydroxy-, 4-carboxy-3-ethyl-5-hydroxyphenyl ester (9CI) (CA INDEX NAME)



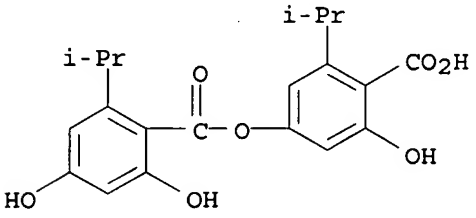
RN 181577-38-8 CAPLUS
CN Benzoic acid, 2,4-dihydroxy-6-methyl-, 4-carboxy-3-hydroxy-5-propylphenyl ester (9CI) (CA INDEX NAME)



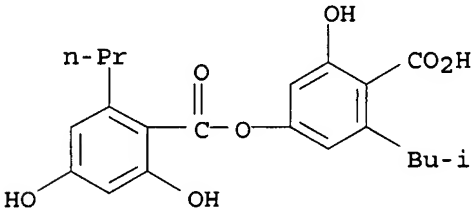
RN 181577-39-9 CAPLUS
CN Benzoic acid, 2,4-dihydroxy-6-propyl-, 4-carboxy-3-hydroxy-5-methylphenyl ester (9CI) (CA INDEX NAME)



RN 181577-41-3 CAPLUS
CN Benzoic acid, 2,4-dihydroxy-6-(1-methylethyl)-, 4-carboxy-3-hydroxy-5-(1-methylethyl)phenyl ester (9CI) (CA INDEX NAME)



RN 181577-42-4 CAPLUS
CN Benzoic acid, 2,4-dihydroxy-6-propyl-, 4-carboxy-3-hydroxy-5-(2-methylpropyl)phenyl ester (9CI) (CA INDEX NAME)

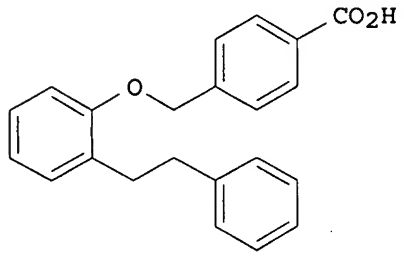


L15 ANSWER 51 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1996:425268 CAPLUS
DN 125:86305
TI Ortho-substituted aromatic ether compounds and their use in pharmaceutical compositions for pain relief
IN Breault, Gloria Anne; Oldfield, John; Tucker, Howard; Warner, Peter
PA Zeneca Limited, UK
SO PCT Int. Appl., 146 pp.

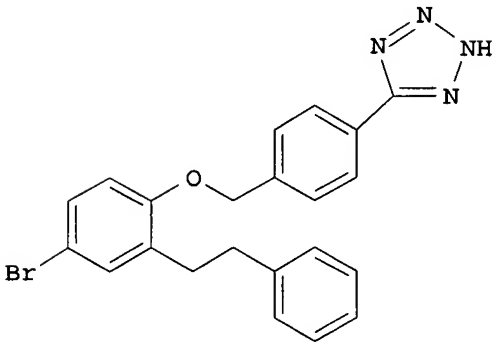
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9606822	A1	19960307	WO 1995-GB2030	19950829
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9533519	A	19960322	AU 1995-33519	19950829
	EP 778821	A1	19970618	EP 1995-929969	19950829
	EP 778821	B1	19991020		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 10504836	T	19980512	JP 1995-508556	19950829
	AT 185791	T	19991115	AT 1995-929969	19950829
	US 5965741	A	19991012	US 1997-793023	19970221
PRAI	GB 1994-17532	A	19940831		
	WO 1995-GB2030	W	19950829		

OS MARPAT 125:86305
GI



I



II

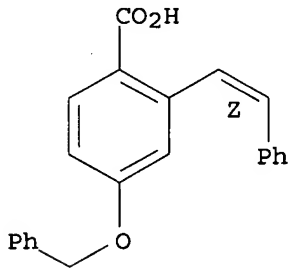
AB The invention relates to compds. of formula D-X-A-O-CH(R3)-B-R' [I; A = (un)substituted ring system; B = (un)substituted 5- or 6-membered heteroaryl or Ph; D = (un)substituted ring system; X = (CHR4)n or (CHR4)pCR4:CR4(CHR4)q wherein n = 1-3 and p and q both = 0, or one of p and q = 1 and the other = 0; R1 = variety of substituents, positioned on ring B in either a 1,3 or 1,4 relationship with the OCH(R3) group for 6-membered rings, or in a 1,3 relationship for 5-membered rings; R3, R4 = H or C1-4 alkyl] as well as their N-oxides, S-oxides, pharmaceutically acceptable salts, and in vivo-hydrolyzable esters and amides. The invention also relates to processes for preparation of I,

intermediates in their preparation, use of I as therapeutic agents, and pharmaceutical compns. containing them. For example, the representative compds. II and III were prepared Benzenoid compound II was prepared via hydrolysis of its Me ester (88%), while tetrazole derivative III was prepared via cycloaddn. of HN3 with the corresponding nitrile (78%). I are analgesics which may also (no data) possess antiinflammatory, antipyretic, and antidiarrheal properties. In general, I had pA2 > 5.3 for inhibiting PGE2-induced contractions of isolated guinea pig ileum, and had oral ED50 of 0.01-100 mg/kg in the phenylbenzoquinone/AcOH induced writhing test in mice. No overt toxicity was seen in the writhing test at several multiples of the min. ED.

IT 178546-76-4P 178546-77-5P 178546-90-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of ortho-substituted aromatic ethers as analgesics)

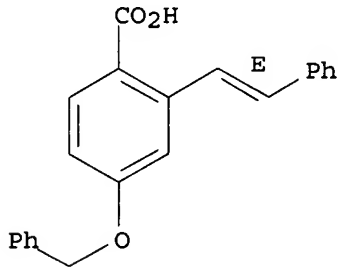
RN 178546-76-4 CAPLUS
CN Benzoic acid, 2-(2-phenylethenyl)-4-(phenylmethoxy)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

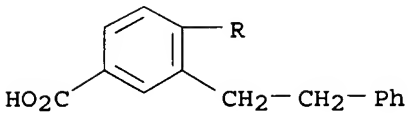


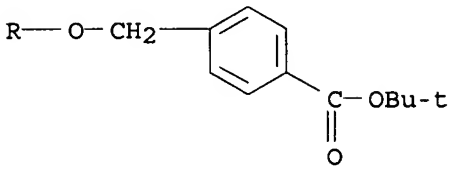
RN 178546-77-5 CAPLUS
CN Benzoic acid, 2-(2-phenylethenyl)-4-(phenylmethoxy)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

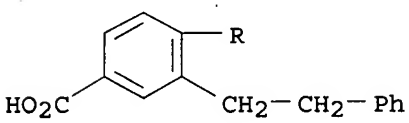


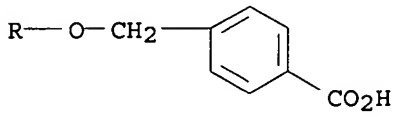
RN 178546-90-2 CAPLUS
CN Benzoic acid, 4-[[4-[(1,1-dimethylethoxy)carbonyl]phenyl]methoxy]-3-(2-phenylethyl)- (9CI) (CA INDEX NAME)





IT 178544-17-7P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of ortho-substituted aromatic ethers as analgesics)
RN 178544-17-7 CAPLUS
CN Benzoic acid, 4-[(4-carboxyphenyl)methoxy]-3-(2-phenylethyl)- (9CI) (CA INDEX NAME)





L15 ANSWER 52 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1996:171786 CAPLUS
DN 124:232070
TI Preparation of substituted fused and bridged bicyclic compound protein kinase C inhibitors
IN Hu, Hong; Jagdmann, G. Erik, Jr.; Mendoza, Jose Serafin
PA Eli Lilly and Co., USA
SO PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9530640	A1	19951116	WO 1995-US3220	19950315
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TT, UA				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 5583221	A	19961210	US 1995-392710	19950223
	CA 2189567	A1	19951116	CA 1995-2189567	19950315

	CA 2189567	C	20060214		
	AU 9519989	A	19951129	AU 1995-19989	19950315
	EP 758312	A1	19970219	EP 1995-913699	19950315
	EP 758312	B1	19991222		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 10500106	T	19980106	JP 1995-528935	19950315
	AT 187956	T	20000115	AT 1995-913699	19950315
	GR 3032950	T3	20000731	GR 2000-400646	20000310
PRAI	US 1994-237645	A	19940504		
	US 1995-392710	A	19950223		
	WO 1995-US3220	W	19950315		

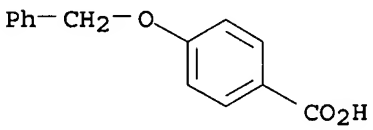
OS MARPAT 124:232070
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; A = (un)substituted NH, O; R1 = H, alkyl; R2-R6 = HO, alkoxy, alkoxycarbonyl, CO2H, CHO, halogen, alkyl, etc.; R7 = H, R2-R6; X = CO, CH2; ring = fused or bridged bicyclic ring optionally containing heteroatoms], useful as inhibitors of protein kinase C and as anticancer and antiinflammatory agents, are prepared and I-containing formulations presented. Thus, indane derivative II, m.p. 160-162°, prepared in a multi-step process from 4-[6-benzyloxy-2-(benzyloxycarbonyl)benzoyl]-3,5-di(benzyloxy)benzoic acid, demonstrated a IC50 of 50 μM against the K562 chronic myeloid leukemia cell line.

IT 1486-51-7, 4-Benzyloxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted fused and bridged bicyclic compound protein kinase C inhibitors)

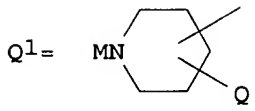
RN 1486-51-7 CAPLUS
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)

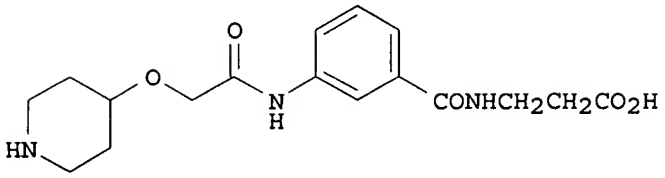


L15 ANSWER 53 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1996:71146 CAPLUS
DN 124:117979
TI Preparation of piperidinyloxyacetylaminobenzoylalanine derivatives and analogs as antithrombotics
IN Kohama, Hiromasa; Kaneda, Shinichi
PA Terumo Corp, Japan
SO Jpn. Kokai Tokkyo Koho, 23 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 07233148	A	19950905	JP 1994-310965	19941214
PRAI	JP 1994-310965	A	19941214		
	JP 1993-332491		19931227		

OS MARPAT 124:117979
GI



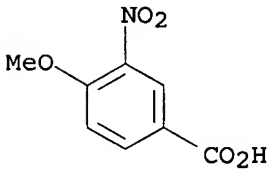


II

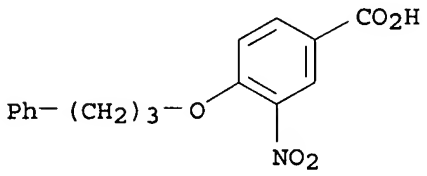
AB The title compds. AOBCONHECONHGCOL (I) [B, G = alkylene; E = phenylene; L = hydroxy, etc.; A = Q1; M, Q = H, alkyl, etc.] are prepared I are GPIIb/IIIa antagonists. β-Alanine derivative II was prepared in a multistep process starting with β-alanine Et ester hydrochloride. II in vitro had IC50 of 0.058 μM against ADP-induced platelet aggregation.

IT 89-41-8P 172899-64-8P 172899-73-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperidinyloxyacetylaminobenzoylalanine derivs. and analogs as antithrombotics)

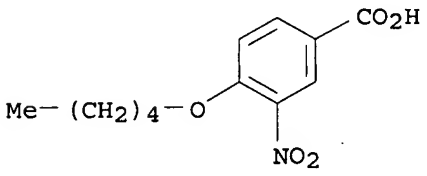
RN 89-41-8 CAPLUS
CN Benzoic acid, 4-methoxy-3-nitro- (CA INDEX NAME)



RN 172899-64-8 CAPLUS
CN Benzoic acid, 3-nitro-4-(3-phenylpropoxy)- (9CI) (CA INDEX NAME)



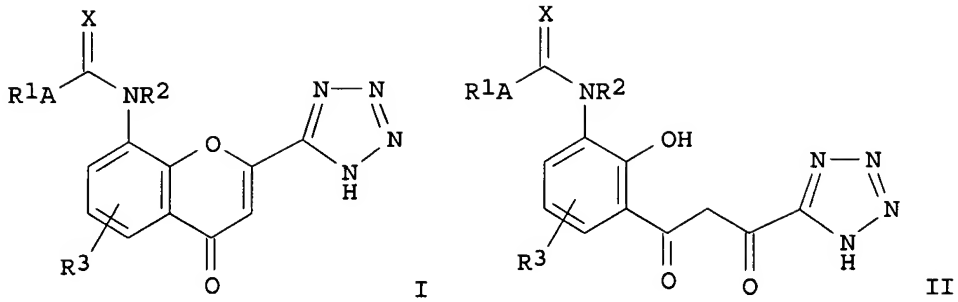
RN 172899-73-9 CAPLUS
CN Benzoic acid, 3-nitro-4-(pentyloxy)- (9CI) (CA INDEX NAME)



L15 ANSWER 54 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:995830 CAPLUS
Correction of: 1994:557653
DN 124:87027
Correction of: 121:157653
TI Cyclization process for preparing tetrazolylbenzopyran compounds
IN Johnson, Graham; smith, Neil; Geen, Rihard Graham; Mann, Inderjit Singh; Novack, Vance
PA SmithKline Beecham PLC, UK
SO PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9412492	A1	19940609	WO 1993-EP3257	19931119
	W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2149886	A1	19940609	CA 1993-2149886	19931119
	CA 2149886	C	20050503		
	AU 9454665	A	19940622	AU 1994-54665	19931119
	AU 673704	B2	19961121		
	EP 670835	A1	19950913	EP 1994-900159	19931119
	EP 670835	B1	20030312		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 08503481	T	19960416	JP 1994-512731	19931119
	JP 3505179	B2	20040308		
	HU 72660	A2	19960528	HU 1995-3137	19931119
	HU 222015	B1	20030328		
	HU 74010	A2	19961028	HU 1995-1553	19931119
	HU 222017	B1	20030328		
	RU 2094428	C1	19971027	RU 1995-113433	19931119
	CZ 282991	B6	19971217	CZ 1997-584	19931119
	CZ 283978	B6	19980715	CZ 1995-1357	19931119
	PL 175039	B1	19981030	PL 1993-309228	19931119
	BR 9307539	A	19990525	BR 1993-7539	19931119
	SK 281083	B6	20001107	SK 1995-696	19931119
	AT 234297	T	20030315	AT 1994-900159	19931119
	ES 2194023	T3	20031116	ES 1994-900159	19931119
	ZA 9308826	A	19950525	ZA 1993-8826	19931125
	IL 107759	A	19981206	IL 1993-107759	19931125
	IL 119366	A	20010826	IL 1993-119366	19931125
	CN 1107153	A	19950823	CN 1993-120531	19931126
	CN 1049657	B	20000223		
	FI 9502585	A	19950526	FI 1995-2585	19950526
	NO 9502090	A	19950529	NO 1995-2090	19950526
	NO 307967	B1	20000626		
	US 5587483	A	19961224	US 1995-451892	19950526
	US 5596103	A	19970121	US 1995-451843	19950526
	US 5616721	A	19970401	US 1995-446666	19950526
	HK 1012393	A1	20031224	HK 1998-113636	19981216
	NO 9906324	A	19950529	NO 1999-6324	19991220
	NO 309718	B1	20010319		
	JP 2004035570	A	20040205	JP 2003-324773	20030917
	JP 3763828	B2	20060405		
PRAI	GB 1992-24922	A	19921127		
	HU 1995-1553	A	19931119		
	JP 1994-512731	A3	19931119		
	WO 1993-EP3257	W	19931119		
	IL 1993-107759	A3	19931125		

OS MARPAT 124:87027
GI

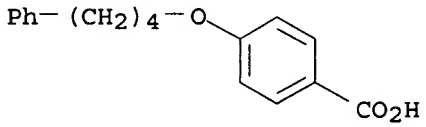


I II

AB The title compds. [I; A = bond, (CH2)n (n = 1-4), CH:CH, etc.; R1 = (un)substituted Ph, naphthyl, C1-20 alkyl, C2-20 alkenyl, etc.; R2 = H, C1-6 alkyl; R3 = H, halo, HO, nitro, (un)substituted CO2H, etc.; X = O, S] are prepared in high yield and purity by the intramol. cyclocondensation of diones II. Thus, to a stirred suspension of NaOMe in dry THF was added 3-[4-(4-phenylbutoxy)benzoylamino]-2-hydroxyacetophenone and Et 5-tetrazolecarboxylate, the mixture stirred at reflux, followed by the addn of concentrated HCl, producing 4-oxo-8-[4-(4-phenylbutoxy)benzoylamino]-2-tetrazol-5-yl-4H-1-benzopyran hemihydrate in 85% yield.

IT 30131-16-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetrazolylbenzopyrans by cyclization of tetrazolecarboxylate with hydroxyacetophenones)

RN 30131-16-9 CAPLUS
CN Benzoic acid, 4-(4-phenylbutoxy)- (CA INDEX NAME)



L15 ANSWER 55 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:835486 CAPLUS
DN 123:257395
TI Imidazolyl amino acid derivatives as angiotensin II antagonists
IN Boyd, Donald B.; Hauser, Kenneth L.; Lifer, Sherryl L.; Marshall, Winston S.; Palkowitz, Alan D.; Pfeifer, William; Reel, Jon K.; Simon, Richard L.; Steinberg, Mitchell I.; et al.
PA Eli Lilly and Co., USA
SO U.S., 29 pp. Cont.-in-part of U.S. Ser. No. 892,867, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

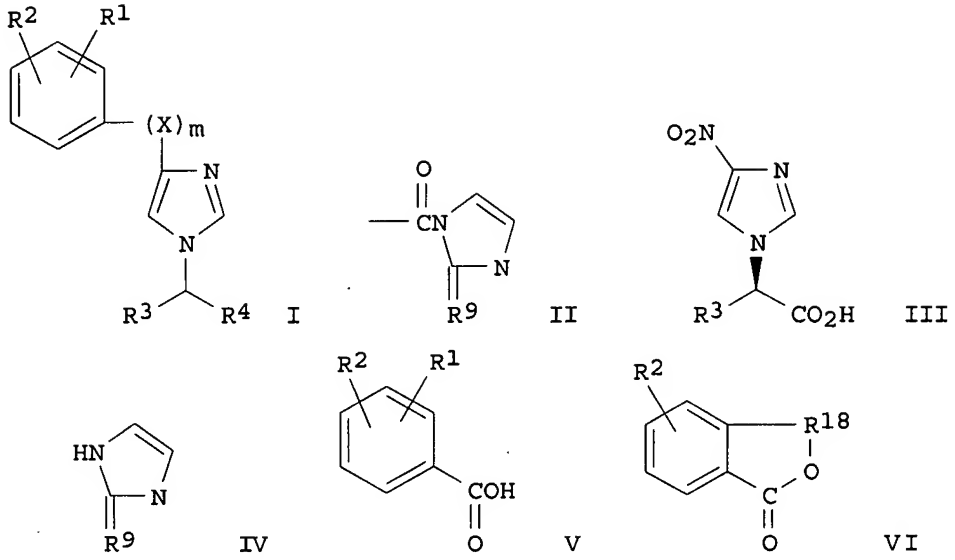
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5401851	A	19950328	US 1993-49917	19930420
	CA 2097462	A1	19931204	CA 1993-2097462	19930601
	HU 64328	A2	19931228	HU 1993-1603	19930601
	IL 105877	A	19980715	IL 1993-105877	19930601
	NO 9302005	A	19931206	NO 1993-2005	19930602
	EP 573271	A1	19931208	EP 1993-304264	19930602

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE

	AU 9339985	A	19940120	AU 1993-39985	19930602
	AU 667903	B2	19960418		
	RU 2110515	C1	19980510	RU 1993-46497	19930602
	CN 1085897	A	19940427	CN 1993-107578	19930603
	CN 1045768	B	19991020		
	JP 07304752	A	19951121	JP 1993-133212	19930603
	PL 173340	B1	19980227	PL 1993-299176	19930603
	US 5484780	A	19960116	US 1994-355778	19941214
PRAI	US 1992-892867	B2	19920603		
	US 1993-49917	A	19930420		

OS CASREACT 123:257395; MARPAT 123:257395

GI



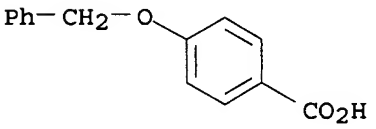
AB A process of preparing a substantially pure (R) enantiomer of the compound of the formula I wherein: R1 is CO2H, SO3H, PO3H2, CONHSO2R5 or 5-tetrazolyl; R2 is H, OH, OCOCH3, halo, C1-C4 alkyl, amino, acetamido, or C1-C4 alkoxy; X is (CH2)mNHCO, (CH2)mCONH, O, NH, CH2, (CH2)mCO, or CO(CH2)m ; R3 is C4-C9 straight chain alkyl, C4-C9 straight chain trifluoroalkyl, C4-C9 straight chain alkenyl, or C4-C9 straight chain trifluoroalkenyl; R4 is CONH(C1-C4 alkyl), CONH(C1-C4 trifluoroalkyl), CONH(hydroxy-C1-C4 alkyl), or, e.g., II; R5 is Ph, C1-C4 alkyl substituted Ph, C1-C5 alkyl, or C1-C5 trifluoroalkyl; R9 is O or S; m is independently 0 or 1; p is independently 0, 1, 2, 3 or 4; and q is 1, 2, 3, or 4 (with provisos); comprising coupling a compound of the formula III to, e.g., IV; reducing the nitro of the compound of the formula III to produce an aminoimidazole; coupling the aminoimidazole to V or VI (R18 = SO2 or CO). Thus, e.g., reaction of 4-nitroimidazole with Et 2-bromooctanoate afforded Et 2-(4-nitro-1H-imidazol-1-yl)octanoate; reaction of the latter with ethylamine afforded N-ethyl-2-(4-nitro-1H-imidazol-1-yl)octanoamide; N-ethyl-2-(4-nitro-1H-imidazol-1-yl)octanoamide was reduced by hydrogenation at 40 psi over Pd/C and the aminoimidazole was added to a solution of 2-sulfobenzoic acid cyclic anhydride to afford N-ethyl-2-[4-(2-sulfobenzoyl)amino-1H-imidazol-1-yl]octanoamide (VII). The ability of I to block angiotensin II receptor binding (KI, μM) was determined using the adrenal glomerulosa assay, and the ability to antagonize angiotensin-induced vasoconstriction [potency = pA2 (defined as -log KB, where KB = [molar concentration of antagonist]/[(EC50 AII with antagonist/EC50 AII without antagonist)-1])] was evaluated in the rabbit aorta test

system: for VII, KI = 10.3 and pA2 = 5.7. Pharmaceutical formulations were given.

IT 1486-51-7, 4-Benzyloxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(imidazolyl amino acid derivs. as angiotensin II antagonists)

RN 1486-51-7 CAPLUS

CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



L15 ANSWER 56 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1995:397335 CAPLUS

DN 122:160476

TI Process of producing 2-cyano-4-oxo-4H-benzopyran compounds.

IN Higashii, Takayuki; Ushio, Hideki; Fujimoto, Yukari; Matsumoto, Tsutomu; Minai, Masayoshi; Yasunaga, Katsuichi; Sogabe, Hiroshi; Kotera, Takahiro

PA Sumitomo Chemical Co., Ltd., Japan

SO Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW

DT Patent

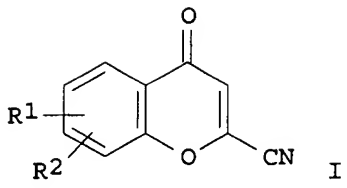
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 634409	A1	19950118	EP 1994-110888	19940713
	EP 634409	B1	20000426		
	R: AT, CH, DE, ES, FR, GB, IT, LI, NL				
	JP 07025819	A	19950127	JP 1993-173333	19930713
	JP 3269188	B2	20020325		
	JP 07025842	A	19950127	JP 1993-174439	19930714
	JP 3185482	B2	20010709		
	JP 07033723	A	19950203	JP 1993-178065	19930719
	JP 3362458	B2	20030107		
	JP 07033759	A	19950203	JP 1993-180250	19930721
	JP 3528204	B2	20040517		
	JP 07053491	A	19950228	JP 1993-207498	19930823
	JP 3486922	B2	20040113		
	JP 07124401	A	19950516	JP 1993-273669	19931101
	JP 3355535	B2	20021209		
	US 5659051	A	19970819	US 1994-273119	19940711
	CA 2127945	A1	19950114	CA 1994-2127945	19940712
	CA 2127945	C	20070109		
	AT 192148	T	20000515	AT 1994-110888	19940713
	ES 2146239	T3	20000801	ES 1994-110888	19940713
PRAI	JP 1993-173333	A	19930713		
	JP 1993-174439	A	19930714		
	JP 1993-178065	A	19930719		
	JP 1993-180250	A	19930721		
	JP 1993-207498	A	19930823		
	JP 1993-273669	A	19931101		

OS CASREACT 122:160476; MARPAT 122:160476

GI



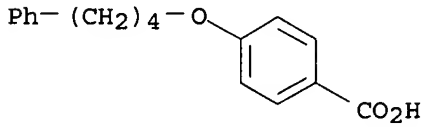
I

AB Title compds. I (R1, R2 = H, halo, HO, C1-4 alkyl, C1-5 alkoxy, O2N, RCONH wherein R = C1-20 alkyl, (substituted)Ph) are prepared by an industrially favorable process by dehydrating (claimed bu not shown)the appropriate 2-carbamoyl-I in presence of a (substituted)pyridine. To 5-ethyl-2-methylpyridine and MeOH was added 8-[4-(4-phenyl-1-butoxy)benzoyl]amino-2-(ethoxycarbonyl)-4-oxo-4H-benzopyran (preparation given) into which NH3(g) was bubbled to give after workup the carbamoyl analog (II). To5-ethyl-2-methylpyridine and MePH was added II at 60° for 6 h to give after workup I (R1 = H, R2 = 8-[4-(4-phenyl-1-butoxy)benzoyl]amino).

IT 30131-16-9P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process of producing 2-cyano-4-oxo-4H-benzopyran compds.)

RN 30131-16-9 CAPLUS

CN Benzoic acid, 4-(4-phenylbutoxy)- (CA INDEX NAME)



L15 ANSWER 57 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1995:229245 CAPLUS

DN 122:9675

TI Preparation of benzoic acid esters as liquid crystals

IN Nishama, Shinichi; Yamaoka, Hideo

PA Mitsui Petrochemical Industries, Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 48 pp.
CODEN: JKXXAF

DT Patent

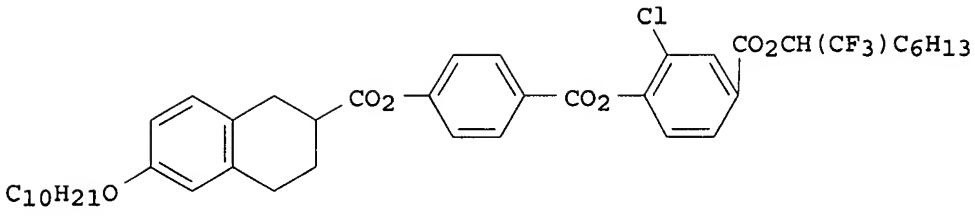
LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 06228056	A	19940816	JP 1993-15002	19930201
PRAI JP 1993-15002		19930201		

OS MARPAT 122:9675

GI



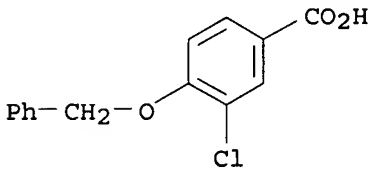
I

AB The title compds. RXA1Y1A2(Y2A3)nCO2R1 [X = CO2, etc.; R = alkyl, etc.; n = 0 or 1; A1 - A3 = divalent aromatic moieties (details on said moieties are given); Y1, Y2 = CO2, etc.; R1 = optically active group] are prepared Ester (R)-I was prepared in a multiple-step process starting with 6-decyloxynaphthalene-2-carboxylic acid. (R)-I showed phase transition temperature of 55° between the SmA-Iso phases.

IT 106931-79-7P 137270-03-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzoic acid esters as liquid crystals)

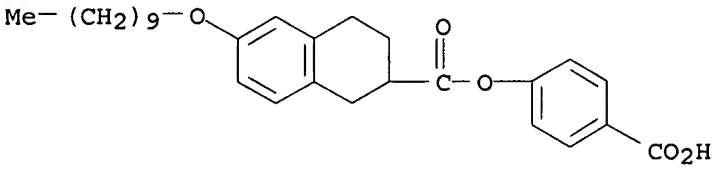
RN 106931-79-7 CAPLUS

CN Benzoic acid, 3-chloro-4-(phenylmethoxy)- (CA INDEX NAME)



RN 137270-03-2 CAPLUS

CN 2-Naphthalenecarboxylic acid, 6-(decyloxy)-1,2,3,4-tetrahydro-, 4-carboxyphenyl ester (9CI) (CA INDEX NAME)



L15 ANSWER 58 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1995:182651 CAPLUS

DN 122:82078

TI Cyclic peptide antifungal agents and process for preparation thereof

IN Burkhardt, Frederick Joseph; Debono, Manuel; Nissen, Jeffrey Scott; Turner, William Wilson, Jr.

PA Eli Lilly and Co., USA

SO Eur. Pat. Appl., 56 pp.
CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	EP 561639	A1	19930922	EP 1993-302064	19930318
	EP 561639	B1	20020515		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	CA 2091663	A1	19930920	CA 1993-2091663	19930315
	ZA 9301830	A	19940915	ZA 1993-1830	19930315
	IL 105048	A	20010614	IL 1993-105048	19930315
	NZ 299314	A	20010928	NZ 1993-299314	19930315
	CZ 288974	B6	20011017	CZ 1993-416	19930315
	IL 122315	A	20020310	IL 1993-122315	19930315
	NZ 512085	A	20030829	NZ 1993-512085	19930315
	NO 9300948	A	19930920	NO 1993-948	19930316
	BR 9301232	A	19930921	BR 1993-1232	19930318
	HU 63637	A2	19930928	HU 1993-785	19930318
	CN 1080926	A	19940119	CN 1993-103587	19930318
	CN 1036715	B	19971217		
	JP 06056892	A	19940301	JP 1993-58529	19930318
	JP 3519754	B2	20040419		
	RU 2129562	C1	19990427	RU 1993-4787	19930318
	AT 217635	T	20020615	AT 1993-302064	19930318
	JP 2002226500	A	20020814	JP 2002-3969	19930318
	JP 3520071	B2	20040419		
	PT 561639	T	20021031	PT 1993-302064	19930318
	ES 2174843	T3	20021116	ES 1993-302064	19930318
	AU 9335341	A	19930923	AU 1993-35341	19930319
	AU 9665529	A	19961205	AU 1996-65529	19960909
	AU 689391	B2	19980326		
	JP 2004115540	A	20040415	JP 2003-412638	20031210
PRAI	US 1992-854117	A	19920319		
	US 1992-992390	A	19921216		
	IL 1993-105048	A3	19930315		
	JP 1993-58529	A3	19930318		

OS MARPAT 122:82078

GI

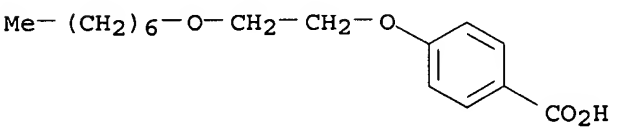
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. (I; R, R11 = independently H, OH; R1 = H, OH, OSO3H; R2 = substituted PhCO, biphenylyl, naphthoyl, etc.; R7 = R1, phosphonooxy; R8 = H, Me, H2NCOCH2; R9, R10 = Me, H), were prepared Thus, I (R = R7 = R11 = OH, R1 = H, R2 = Q1, R8 = R9 = R10 = Me), prepared by enzymic deacylation and then reacylation of echinocandin B, showed ED50 = 0.84 mg/mL for controlling systemic fungal infections in mice. Several I were effective against Pneumocystis carinii in immunosuppressed rats. I in general exhibit oral bioavailability.

IT 158938-01-3P 158938-02-4P 158938-03-5P
158938-04-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for cyclic peptide deriv medical fungicide)

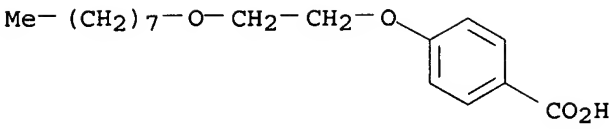
RN 158938-01-3 CAPLUS

CN Benzoic acid, 4-[2-(heptyloxy)ethoxy]- (9CI) (CA INDEX NAME)

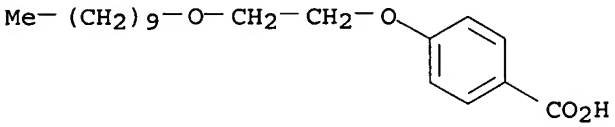


RN 158938-02-4 CAPLUS

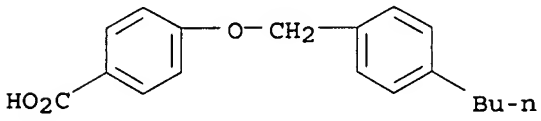
CN Benzoic acid, 4-[2-(octyloxy)ethoxy]- (9CI) (CA INDEX NAME)



RN 158938-03-5 CAPLUS
CN Benzoic acid, 4-[2-(decyloxy)ethoxy]- (9CI) (CA INDEX NAME)



RN 158938-04-6 CAPLUS
CN Benzoic acid, 4-[(4-butylphenyl)methoxy]- (9CI) (CA INDEX NAME)

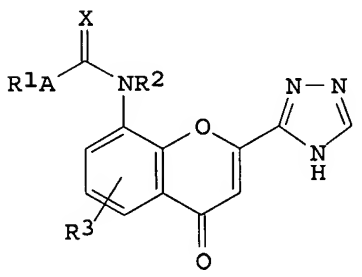


L15 ANSWER 59 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1994:557653 CAPLUS
DN 121:157653
TI Cyclization process for preparing tetrazolylbenzopyran compounds
IN Johnson, Graham; Smith, Neil; Geen, Richard Graham; Mann, Inderjit Singh; Novack, Vance
PA Smithkline Beecham PLC, UK
SO PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DT Patent
LA English

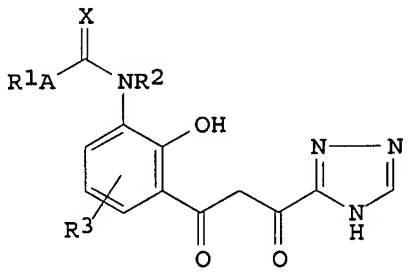
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9412492 A1		19940609	WO 1993-EP3257	19931119

W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

PRAI GB 1992-24922 19921127
OS CASREACT 121:157653; MARPAT 121:157653
GI



I



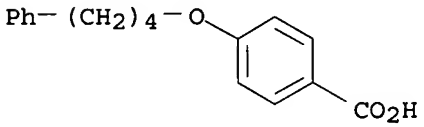
II

AB The title compds. [I; A = direct bond, methylene, ethylene, trimethylene, tetramethylene, vinylene, etc.; R1 = (un)subsitituted Ph, 2-naphthyl, C1-20 alkyl, C2-20 alkenyl, etc.; R2 = H, C1-6 alkyl; R3 = H, halogen, OH, NO2, (un)substituted CO2H, etc.; X = O, S] are prepared in high yield and purity by the intramol. cyclocondensation of dione II. Thus, to a stirred suspension of NaOMe in dry THF was added 3-[4-(4-phenylbutoxy)benzoylamino]-2-hydroxyacetophenone and Et 5-tetrazolecarboxylate, the mixture stirred at reflux, followed by the addition of concentrated HCl, producing 4-oxo-8-[4-(4-phenylbutoxy)benzoylamino]-2-tetrazol-5-yl-4H-1-benzopyran hemihydrate in 85% yield.

IT 30131-16-9P, 4-(4-Phenylbutoxy)benzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of benzopyrans)

RN 30131-16-9 CAPLUS

CN Benzoic acid, 4-(4-phenylbutoxy)- (CA INDEX NAME)



L15 ANSWER 60 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1992:193997 CAPLUS

DN 116:193997

TI New approaches to pyrrolo[2,1-c][1,4]benzodiazepines: synthesis, DNA-binding and cytotoxicity of DC-81

AU Rose, D. Subhas; Jones, Gary B.; Thurston, David E.

CS Sch. Pharm. Biomed. Sci., Portsmouth Polytech., Portsmouth/Hants., PO1 2DZ, UK

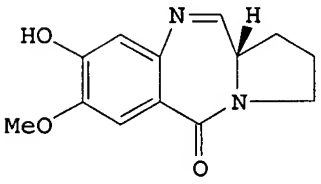
SO Tetrahedron (1992), 48(4), 751-8
CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

OS CASREACT 116:193997

GI



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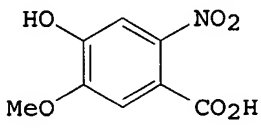
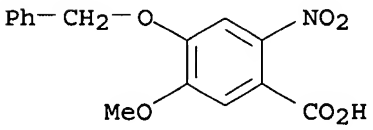


II

AB Two routes to the naturally occurring DNA-binding antitumor antibiotic DC-81 (I) are described, one of which involves a novel cyclization process based on acid resin. The second route involves the synthesis of a new compound, 6-nitrovanillic acid (II), a key A-ring component of many naturally occurring title compds. These routes have provided a sufficient quantity of DC-81 to allow complete characterization and evaluation in DNA-binding and in vitro cytotoxicity studies.

IT 60547-92-4
RL: RCT (Reactant); RACT (Reactant or reagent)

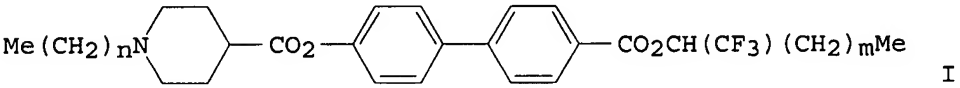
(amidation and debenzylation of)
RN 60547-92-4 CAPLUS
CN Benzoic acid, 5-methoxy-2-nitro-4-(phenylmethoxy)- (CA INDEX NAME)



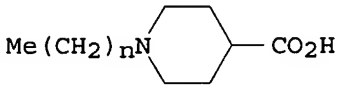
L15 ANSWER 61 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1991:461003 CAPLUS
DN 115:61003
TI Optically-active 4'-(1-trifluoromethylalkoxycarbonyl)-4-biphenylyl N-alkylisonipecotinates as tristable ferroelectric liquid crystals and their preparation
IN Aihara, Yoshihiko; Numazawa, Koichi; Sakuma, Shigenori
PA Showa Shell Sekiyu K. K., Japan
SO Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 02270862	A	19901105	JP 1989-90775	19890412
JP 2853044	B2	19990203		
PRAI JP 1989-90775		19890412		

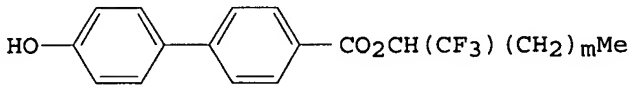
OS MARPAT 115:61003
GI



I



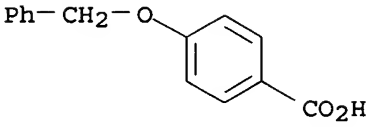
II



III

AB The title esters I (m = 4-11; n = 4-13) as liquid crystals and a process for the preparation of I by dehydration-condensation of N-alkylisonipecotinic acids II with 4'-substituted-4-hydroxybiphenyls III are claimed. I are novel ferroelec. liquid crystals showing tristable states and the use of I simplify the matrix of display devices. A THF solution of 0.32 g II (n = 7) and 0.38 g III (m = 5) was treated with DCC and dimethylaminopyridine at room temperature for 10 h to give 0.08 g I (m = 5, n = 7), showing a chiral smectic C phase and tristability.
IT 1486-51-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acid chlorination of, in preparation of tristable ferroelec.
liquid crystal)
RN 1486-51-7 CAPLUS

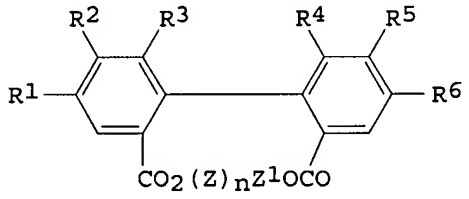
CN Benzoic acid, 4-(phenylmethoxy)- (CA INDEX NAME)



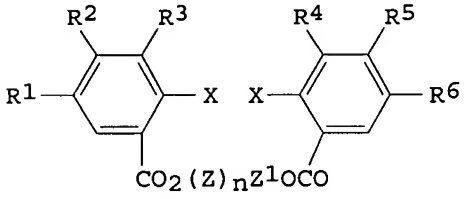
L15 ANSWER 62 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1991:228973 CAPLUS
DN 114:228973
TI Biphenyl-2,2'-dicarboxylic acid cyclic esters for treatment of liver diseases, their intermediates, and their preparations
IN Iwasaki, Tameo; Kondo, Kazuhiko; Matsuoka, Yuzo; Matsumoto, Mamoru; Sugiura, Masaki
PA Tanabe Seiyaku Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 03011076	A	19910118	JP 1989-141989	19890602
	JP 06013502	B	19940223		
PRAI	JP 1989-141989		19890602		

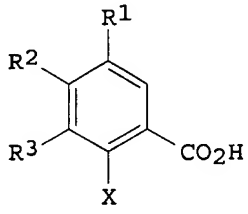
OS MARPAT 114:228973
GI



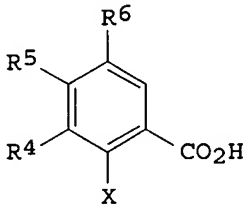
I



II



III



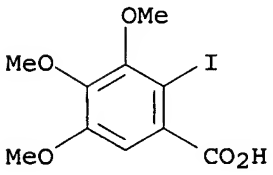
IV

AB The title compds. I (R1 - R6 = H, lower alkoxy, lower phenylalkoxy; vicinal 2 of them may be bonded to form lower alkylenedioxy; 1 or 2 of R1 - R6 = H; Z = arylene, Z1 = lower alkylene, n = 0, 1), a process for the preparation of I by intramol. cyclization, of bis(halophenyl) compds. II (X = halo), a process for the preparation of II by treatment of

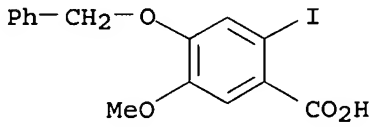
HOZ1ZnOH or their salts with halobenzoic acids III and IV, their carboxy-reactive derivs., or their salts, and II are claimed. An AcNMe2 suspension of 62.1 g 2-iodo-3,34-methylenedioxybenzoyl chloride (preparation given) was added dropwise to a mixture of salicyl alc. (22.4 g), Et3N, 4-dimethylaminopyridine, and AcNMe2 at ≤-25° and the reaction mixture was stirred at -25° for 30 min, gradually heated, further stirred at room temperature for 5 h. Subsequently an AcNMe2 suspension of 52.8 g 2-iodo-3,4-dimethoxybenzoyl chloride (preparation given) was added at -30° and the reaction mixture was further stirred at room temperature overnight to give 89.4 g 2-iodo-3,4-methylenedioxybenzoic acid [2-[(2-iodo-4,5-dimethoxyphenyl)carbonyloxy]benzyl] ester. This (89.5 g) in DMF was added dropwise to DMF containing Cu under reflux over 3 h and the reaction mixture was further refluxed for 2 h to give 53.7 g 5,6-methylenedioxy-4',5'-dimethoxy-2'-(2-hydroxymethylphenyloxycarbonyl)-2-biphenylcarboxylic acid lactone (V). V at 100 mg/kg. p.o. inhibited CCl4-induced increase of GTP (glutamic-pyruvic transaminase) activity in mice ≥20%.

IT 98799-41-8, 2-Iodo-3,4,5-trimethxoybenzoic acid
133681-92-2, 4-Benzyloxy-2-iodo-5-methoxybenzoic acid
133682-07-2 133682-08-3, 4,5-Diethoxy-2-iodobenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of)

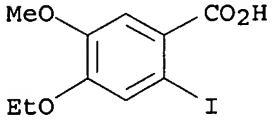
RN 98799-41-8 CAPLUS
CN Benzoic acid, 2-iodo-3,4,5-trimethoxy- (CA INDEX NAME)



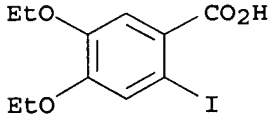
RN 133681-92-2 CAPLUS
CN Benzoic acid, 2-iodo-5-methoxy-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



RN 133682-07-2 CAPLUS
CN Benzoic acid, 4-ethoxy-2-iodo-5-methoxy- (9CI) (CA INDEX NAME)



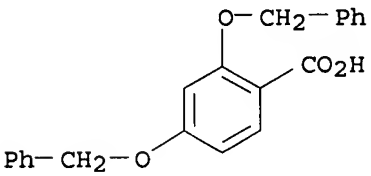
RN 133682-08-3 CAPLUS
CN Benzoic acid, 4,5-diethoxy-2-iodo- (9CI) (CA INDEX NAME)



L15 ANSWER 63 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:478592 CAPLUS
DN 111:78592
TI Preparation of N-β-alanyl-N'-(N-2,4-dihydroxyphenylacetyl-L-asparagyl)cadaverine derivatives as glutamic acid receptor inhibitors and process and intermediate thereof
IN Nakajima, Terumi; Kawai, Nobumi; Shudo, Koichi; Shiba, Tetsuo
PA Takeda Chemical Industries, Ltd., Japan; Zaidan Hojin Tokyoto Shinkei Kagaku Sogyo Kenkyusho
SO Jpn. Kokai Tokkyo Koho, 17 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 63310856	A	19881219	JP 1987-145667	19870610
	JP 07088343	B	19950927		
PRAI	JP 1987-145667		19870610		

OS MARPAT 111:78592
AB QNHCH(CH2CH2CONH2)CONH(CH2)5NHCO(CH2)2NH[(CH2)mNH]pNH(CH2)nNHR [I; Q = 2,4-(HO)2C6H3CH2CO; R = H, COCH(NH2)(CH2)3NHC(:NH)NH2 (Q1); m, n = 3,4; p = 0,1] were prepared as glutamic acid receptor inhibitors. Coupling of 2,4-(PhCH2O)2C6H3CH2CO-Asn-NH(CH2)5NHR.AcOH [R = H2N(CH2)4NZCH2CH2CO where Z = CO2CH2Ph] with Z-Arg(Z2)-OH [L-ZNHC(:NH)NZ(CH2)3CH(NHZ)CO2H] via a mixed anhydride with iso-BuO2CCl in DMF/THF containing Et3N at -20° and then 20° gave, after hydrolgenolysis over Pd black in MeOH, 2,4-(HO)2C6H3CH2CO-Asn-NH(CH2)5NHR [II; R = H-Arg-NH(CH2)4NHCH2CH2CO].
IT 85593-77-7P, 2,4-Dibenzyloxybenzoic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for glutamic acid receptor inhibitor)
RN 85593-77-7 CAPLUS
CN Benzoic acid, 2,4-bis(phenylmethoxy)- (CA INDEX NAME)



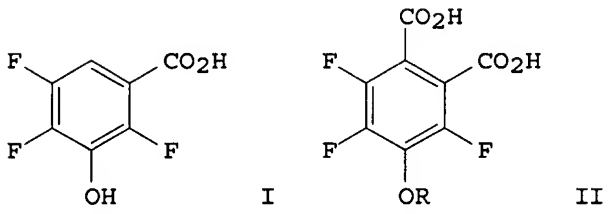
L15 ANSWER 64 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1988:570038 CAPLUS
DN 109:170038
TI 2,4,5-Trifluoro-3-hydroxybenzoic acid, useful as an intermediate for quinolone carboxylate antibacterials such as ofloxacin, and a process for its preparation
IN Ataka, Kikuo; Oku, Masayoshi
PA Ube Industries, Ltd., Japan
SO Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 271275	A1	19880615	EP 1987-310569	19871201
	EP 271275	B1	19911127		
	R: CH, DE, FR, GB, IT, LI				
	US 4831190	A	19890516	US 1987-126173	19871127
	JP 63264440	A	19881101	JP 1987-303312	19871202

	JP 07078033	B	19950823		
	JP 63264439	A	19881101	JP 1987-303313	19871202
	JP 06096545	B	19941130		
PRAI	JP 1986-287763	A	19861204		
	JP 1986-290399	A	19861208		

OS CASREACT 109:170038; MARPAT 109:170038

GI



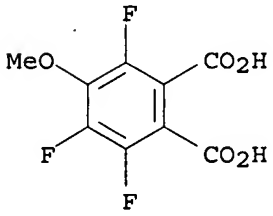
I II

AB The title acid (I), useful as an intermediate for quinolone antibacterials such as ofloxacin, is prepared by hydrolysis-decarboxylation of trifluorohydroxyphthalic acid derivs. II (R = H, hydrolyzable organic group). 3,4,5,6-Tetrafluorophthalic acid was heated in aqueous KOH at 90° for 9 h to give 98% II (R = H). This compound was heated in H2O under N at 140° (sealed tube) for 3 h to give 90% I.

IT 28889-41-0, 3,5,6-Trifluoro-4-methoxyphthalic acid
116751-28-1, 3,5,6-Trifluoro-4-ethoxyphthalic acid
116751-29-2, 3,5,6-Trifluoro-4-propoxyphthalic acid
116751-30-5, 3,5,6-Trifluoro-4-butoxyphthalic acid
116751-31-6, 3,5,6-Trifluoro-4-benzyloxyphthalic acid
116751-32-7, 3,5,6-Trifluoro-4-acetoxyphthalic acid
116751-33-8, 3,5,6-Trifluoro-4-benzoyloxyphthalic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis-decarboxylation of)

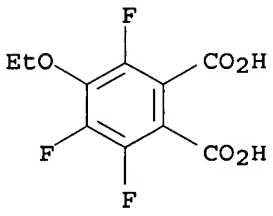
RN 28889-41-0 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 3,4,6-trifluoro-5-methoxy- (9CI) (CA INDEX NAME)



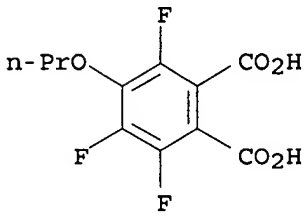
RN 116751-28-1 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 4-ethoxy-3,5,6-trifluoro- (9CI) (CA INDEX NAME)

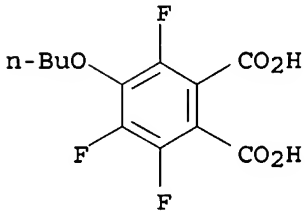


RN 116751-29-2 CAPLUS

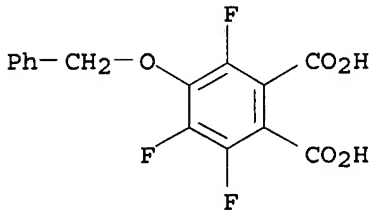
CN 1,2-Benzenedicarboxylic acid, 3,4,6-trifluoro-5-propoxy- (9CI) (CA INDEX NAME)



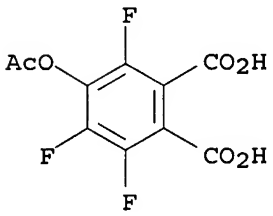
RN 116751-30-5 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 4-butoxy-3,5,6-trifluoro- (9CI) (CA INDEX NAME)



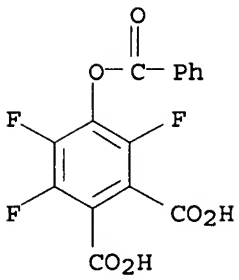
RN 116751-31-6 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3,4,6-trifluoro-5-(phenylmethoxy)- (9CI) (CA INDEX NAME)



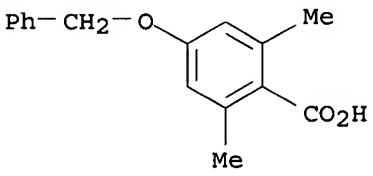
RN 116751-32-7 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 4-(acetyloxy)-3,5,6-trifluoro- (9CI) (CA INDEX NAME)



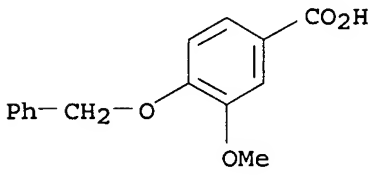
RN 116751-33-8 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 4-(benzoyloxy)-3,5,6-trifluoro- (9CI) (CA INDEX NAME)



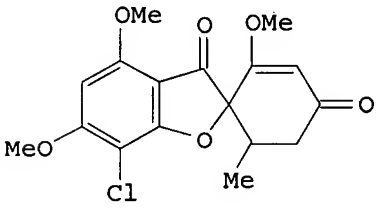
L15 ANSWER 65 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1985:220246 CAPLUS
DN 102:220246
TI Reactivity in the para oxo ketene route of ester hydrolysis. The effect of internal nucleophilicity and the irrelevance of B strain
AU Thea, Sergio; Cevasco, Giorgio; Guanti, Giuseppe; Kashefi-Naini, Nasrin; Williams, Andrew
CS Ist. Chim. Org., Univ. Genova, Genoa, Italy
SO Journal of Organic Chemistry (1985), 50(11), 1867-72
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 102:220246
AB The hydrolysis of 2,4-dinitrophenyl esters of substituted 4-hydroxybenzoic acids obeys the equation kobsd = (ka + kb[OH-])/(1 + [H+]/Ka) and involves a para oxo ketene intermediate. The ka term fits a Broensted equation against the pK of the 4-hydroxybenzoate (log ka = 1.15pKa - 11.71) provided the 2,6-positions of the benzoate are free. The ka term for the 2,6-dimethyl-4-hydroxybenzoate ester is 1015-fold larger than that for the parent 4-hydroxybenzoate ester. An electronic effect due to different hydroxyl pKa's may be calculated from the above linear free energy relationship to contribute 1.6% of the discrepancy. The other component of the discrepancy is ascribed to a preferred alignment of the ester in the 2,6-di-Me case perpendicular to the plane of the aromatic ring. The fused ketene in the microscopic reverse reaction has a LUMO acceptor orbital perpendicular to the plane of the ring in agreement with these conclusions. Force-field calcns. of nonbonding interactions indicate no strain release in the elimination mechanism giving rise to ka. The dramatic (107-fold) enhancement of the apparent second-order rate constant for alkaline hydrolysis of the 2,6-di-Me ester, compared with that of the corresponding 2,4-dinitrophenyl 4-methoxy-2,6-dimethylbenzoate, is due mostly to the steric strain imposed in the tetrahedral transition state for the latter reaction. This strain is not sufficient, however, to cause the normal BAc2 mechanism in the alkaline hydrolysis of mesitoates to change to a square planar concerted process.
IT 95741-45-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 95741-45-0 CAPLUS
CN Benzoic acid, 2,6-dimethyl-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



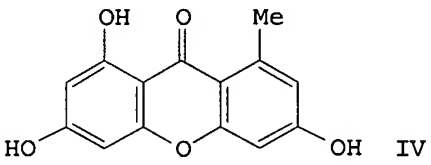
L15 ANSWER 66 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1983:18276 CAPLUS
DN 98:18276
TI Synthesis of lignin model dimers by novel techniques
AU Dimmel, Donald R.; Shepard, Donaline
CS Inst. Paper Chem., Appleton, WI, 54912, USA
SO Journal of Wood Chemistry and Technology (1982), 2(3), 297-315
CODEN: JWCTDJ; ISSN: 0277-3813
DT Journal
LA English
AB A procedure, involving the selective alkylation of β-C of an unprotected phenolic β-aryl ether α-keto compound followed by reduction with NaBH4 and treatment with AcCl, was developed for the synthesis of β-aryl ether models, such as 1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)ethanol [7382-68-5], capable of generating quinonemethides in alkaline solns. The alkylation process was limited to simple electrophiles, and the attempts to prepare α-hydroxy-β-aryl ether lignin models by stereospecific ring openings of styrene (I) and substituted I failed.
IT 1486-53-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 1486-53-9 CAPLUS
CN Benzoic acid, 3-methoxy-4-(phenylmethoxy)- (CA INDEX NAME)



L15 ANSWER 67 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1976:519401 CAPLUS
DN 85:119401
TI Biosynthesis of griseofulvin
AU Harris, Constance M.; Roberson, Jill S.; Harris, Thomas M.
CS Dep. Chem., Vanderbilt Univ., Nashville, TN, USA
SO Journal of the American Chemical Society (1976), 98(17), 5380-6
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
GI



I



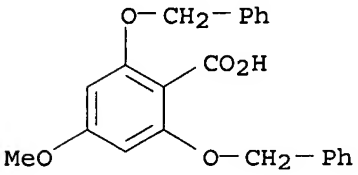
IV

AB The antifungal antibiotic griseofulvin (I) is a polyketide metabolite of Penicillium griseofulvum [patulum]. There are ≤ 2 and probably 3 O-Me groups which are introduced after both carbocyclic rings are formed. 2,4,4',6-Tetrahydroxy-2'-methoxy-6'-methylbenzophenone, the monomethylated precursor predicted by earlier workers, was not detected in cultures by

carrier dilution expts. Instead 2,2',4',6-tetrahydroxy-4-methoxy-6'-methylbenzophenone (II) is a precursor of I as indicated by a feeding experiment in which II containing a tritium label in the O-Me group was incorporated (14%) into I. Demethylation of labeled I 1st to griseofulvic acid and then to grisan showed that < 10% randomization of the label occurred during biotransformation of II into I. The possibility that nonmethylated 2,2',4,4',6-pentahydroxy-6'-methylbenzophenone (III) was the precursor of II was considered, but synthetic III was too unstable for use in carrier dilution or incorporation expts., undergoing facile cyclization to xanthone (IV). The latter compound was, however, a metabolite of P. griseofulvum, which lends support to the hypothesis that both II and IV arise in the fungal culture from III. Earlier workers had postulated that the grisan ring is formed by oxidative cyclization of griseophenone A to give dehydrogriseofulvin but in vivo confirmation of this process has not been obtained. Another possible precursor to dehydrogriseofulvin, normethyldehydrogriseofulvin was synthesized and incorporated (44%) into I. These findings support the biosynthetic sequence: acetate → heptaacetic acid → III → II → griseophenone C → griseophenone B → normethyldehydrogriseofulvin → dehydrogriseofulvin → I.

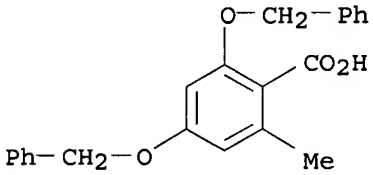
IT 60556-51-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with bis(benzyloxy)toluene)

RN 60556-51-6 CAPLUS
CN Benzoic acid, 4-methoxy-2,6-bis(phenylmethoxy)- (9CI) (CA INDEX NAME)

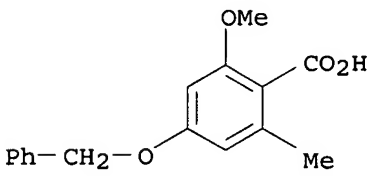


IT 7141-98-2P 22375-06-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with tris(benzyloxy)benzene)

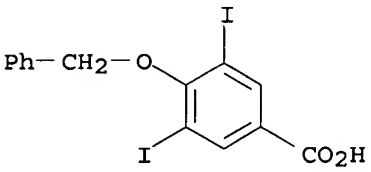
RN 7141-98-2 CAPLUS
CN Benzoic acid, 2-methyl-4,6-bis(phenylmethoxy)- (9CI) (CA INDEX NAME)



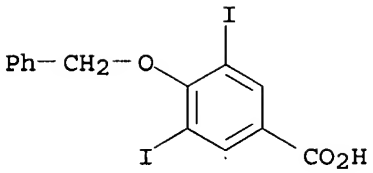
RN 22375-06-0 CAPLUS
CN Benzoic acid, 2-methoxy-6-methyl-4-(phenylmethoxy)- (CA INDEX NAME)



L15 ANSWER 68 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1965:61903 CAPLUS
DN 62:61903
OREF 62:11011g-h
TI Effect of 4-benzylhydroxy-3,5-diiodobenzoic acid on the oxidative phosphorylation of liver and tumor mitochondria
AU Bacigalupo, G.; Wand, H.
CS Deut. Akad. Wiss., Berlin
SO Experientia (1964), 20(10), 578-9
CODEN: EXPEAM; ISSN: 0014-4754
DT Journal
LA German
AB The s.c. transplanted Walker carcinoma sarcoma 256 was removed from 10 200-g. rats 10 days later and homogenized in 0.25M sucrose and 0.001M EDTA. Simultaneously, the liver was removed from the same rats and similarly treated. The mitochondria from both sources were isolated and the P:O ratio was determined Samples, (200 mg. from liver, 400 mg. from the sarcoma) were placed in a complex medium to which concns. of 10-6 to 10-4M 4-benzylhydroxy-3,5-diiodobenzoic acid (I) were added. After 15 min. at 30° data for respiration and phosphorylation were recorded and plotted. The plots show that the respiration and phosphorylation data were reduced in both types of mitochondria in the presence of I; but the effect was far greater in the sarcoma than in the liver of the same rats.
IT 842-35-3, Benzoic acid, 4-(benzyloxy)-3,5-diiodo-
(in phosphorylation by liver and neoplasm mitochondria)
RN 842-35-3 CAPLUS
CN Benzoic acid, 3,5-diiodo-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



L15 ANSWER 69 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1964:419252 CAPLUS
DN 61:19252
OREF 61:3323h,3324a-b
TI Effects of 4-benzyloxy-3,5-diiodobenzoic acid on the oxidative phosphorylation of isolated mitochondria
AU Wand, H.; Bacigalupo, G.
CS German Acad. Sci., Berlin-Buch
SO Nature (London, United Kingdom) (1964), 022(4929), 295-6
CODEN: NATUAS; ISSN: 0028-0836
DT Journal
LA Unavailable
AB At a concentration of 10-4M, 4-benzyloxy-3,5-diiodobenzoic acid (BIBA) caused complete inhibition of phosphorylation and a slight inhibition of respiration. Decreased P/O ratio and partial inhibition of respiration were found with nicotinamide adenine dinucleotide (NAD)-linked substrates such as glutamate and ketoglutarate and with NAD-independent succinate. BIBA, like dinitrophenol (DNP), induced a high rate of respiration in mitochondria that had been incubated in absence of hexokinase and a phosphate aceeptor. BIBA caused a marked inhibition of DNP-stimulated adenosine triphosphatase. In the presence of amytal and of high concns. of BIBA, almost complete depression of DNP-stimulated adenosine triphosphatase occurred.
IT 842-35-3, Benzoic acid, 4-(benzyloxy)-3,5-diiodo-
(mitochondrial response to)
RN 842-35-3 CAPLUS
CN Benzoic acid, 3,5-diiodo-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



L15 ANSWER 70 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1964:3146 CAPLUS
DN 60:3146
OREF 60:517b-h,518a-h
TI Tumor chemotherapy. XIV. Synthesis of compounds related to actinomycins. Derivs. of 2-amino-3-phenoxazone
AU Chao, Shu-Wei; Kao, Yee-Sheng; Chou, Ching-Hsu; Hsu, Bin
CS Acad. Sinica, Shanghai, Peop. Rep. China
SO Scientia Sinica (English Edition) (1963), 12(1), 49-71
CODEN: SSINAV; ISSN: 0582-236X
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB cf. CA 60, 444b. The title derivs. were screened against S180 and Ehrlich ascites carcinoma in mice. Some of the compds. possess a moderate degree of inhibition against the said experimental tumors, given by intraperitoneal injection, but the action reverses to a stimulating effect upon oral administration. The compds. were prepared by the oxidative condensation of the corresponding o-aminophenol. 2-Nitro-3-methoxy-4-hydroxybenzaldehyde (I) (10 g.) is oxidized with fresh Ag2O to give 9.5 g. crude 2-nitro-3-methoxy-4-hydroxybenzoic acid (II), m. 257° (aqueous alc.); Me ester m. 181-2.5° (aqueous MeOH). II (0.02 mole) in 22 ml. 2N KOH to which Me2SO4 (6 ml.) is added gradually at room temperature was heated on the water bath while maintaining the solution alkaline by the occasional addition of 2N KOH. Then 8 ml. 6N KOH was added and heating continued till the oil dissolved. The mixture was filtered and acidified to give 2-nitro-3,4-dimethoxybenzoic acid (III), m. 202-3.5°, in 90% yield. Similarly, II was converted into 2-nitro-3-methoxy4-ethoxybenzoic acid (IV), m. 192-3°, with Et2SO4. II treated with MeOH-KOH-iso-PrI gave 2-nitro-3-methoxy-4-isopropoxybenzoic acid (V), m. 173.5-4.5° (aqueous alc.). II was similarly treated with benzyl chloride to give 2-nitro-3-methoxy-4-benzyloxybenzoic acid (VI), m. 182-3°. I treated with MeOH-KOHiso-PrI gave 2-nitro-3-methoxy-4-isopropoxybenzaldehyde, m. 83.5-4.5°(alc.), which was oxidized to V with Ag2O. The following 2-nitro-3-ethoxy-4-substituted benzoic acids (VIIa-d) were obtained by treating the corresponding 2-nitro-3-hydroxy-4-substituted benzoic acids (VIIIa-d) with Et2SO4 and excess alkaline (substituent and m.p. of VII given) VIIa, OMe, 198-9°; VIIb, OEt, 166-7°; VIIc, Me, 182.5-3.5°; VIId, H, 207.5-8.5°. III (3 g.) heated at 130-5° with 95 ml. 48% HBr until solution occurred was selectively demethylated to VIIIa, m. 229° (decomposition) (aqueous alc.), in 66% yield. VIIIa was obtained quant. by refluxing a mixture of 34 g. III and 108 g. KOH in 250 ml. H2O at 150-60° for 4 hrs. VIIIb, m. 219.5° (decomposition), and VIIIc, m. 185-6°, were prepared from the alkaline treatment of IV and of 2-nitro-3-methoxy-p-toluic acid, in about 90% yield. However, alkaline treatment of V and VI was unsuccessful, and similarly attempted deethylation of VIIa-c failed, but VIId gave VIIId. VIIIa-d were dibenzylated with MeOH-KOH-benzyl chloride followed by alkaline hydrolysis to give the corresponding 2-nitro-3-benzyloxy-4-substituted benzoic acids (IXa-d), m. 186-7°, 181-2.5°, 175-6°, 193-4°, resp. Thus, VIIIa 25 treated with KOH 15 in MeOH 125 and benzyl chloride 31 parts was stirred on the water bath for

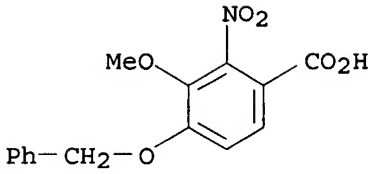
more than 10 hrs. NaOH 20 in H2O 125 parts was added and the mixture heated and stirred till solution was complete. Steam distillation, acidification of the residue to pH 2, cooling, filtration, and thorough H2O washing gave 90% (crude) IXa, m. 186-7° (aqueous alc.). The intermediate dibenzylated product, e.g., 2-nitro-3-benzyloxy-4-methoxybenzoic acid benzyl ester, m. 83.5-4.5° (alc.), from VIIIa could be isolated, which was then hydrolyzed to IXa with aqueous NaOH. IXc and IXd were similarly prepared from 2-nitro-3-benzyloxy-4-methylbenzoic acid benzyl ester, m. 96-7° (C6H6), and 2-nitro-3-benzyloxybenzoic acid benzyl ester, m. 83-83.5° (alc.). VIIIa Me ester, m. 170-1° (MeOH), was benzylated to 2-nitro-3-benzyloxy-4-methoxybenzoic acid Me ester, m. 96-7° (MeOH), and hydrolyzed to IXa with dilute NaOH. IXa-d were converted into the corresponding acid chlorides (Xa-d), m. 122.5-4°, 114-16%, 109-11.5°, and 93-4°, in 92-95% yield by treating a suspension of the acid in CHCl3 with an equal weight of PCl6 below 50° until solution was complete. Xa was treated with glycine (XIa), β-alanine (XIb) and 1-aminocyclopentane-1-carboxylic acid (XIc) to give the corresponding 2-nitro-3-benzyloxy-4-methoxybenzoylamino acids (XIIa-c), m. 155-6°, 168-9°, and 203.5-4.5°, resp. Thus, a solution of 0.01 mole Xa in 15 ml. dry tetrahydrofuran (THF) and another solution of 5 ml. 2N NaOH were added dropwise simultaneously to a solution of 0.011-0.012 mole XI in 13 ml. 2N NaOH and 10 ml. THF at a rate to maintain the pH at 8-9. After the addition, the mixture was stirred at room temperature for 1.5 hrs. and then acidified with dilute HCl. The solvent was removed in vacuo, and the product separated by filtration. The crude product (quant. yield) was recrystd. from aqueous alc. to give pure XII. Xa (0.01 mole) dissolved in THF (1 g. Xa; 5 ml. THF) and a solution of 5 ml. 2N NaOH was added separately to a solution of 0.011 mole of the hydrochloride of XI ethyl esters (1 g.: 5 ml. 1:1 THF-H2O) which had been previously neutralized with 5 ml. 2N NaOH (ice-cooling). After stirring for an addnl. 0.5 hour, and left at room temperature for an hour, the THF was removed in vacuo. The solid was filtered off and washed with H2O to give the crude product in quantitative yield. The product was recrystd. from alc. Thus, Xa was treated with XIa-c Et ester hydrochlorides (XIIIa-c) and phenylalanine Et ester hydrochloride (XIIId) to give the corresponding 2-nitro-3-benzyloxy-4 methoxybenzoylamino acid Et ester (XIVa-d), resp., m. 113.5-14.5°, 105.6-6.5°, 157.5-8.5°, and 163-4°. Similarly, from Xb and XIIIa was obtained XIVe, m. 100.5-1.5°; from Xc and XIIIa-d were obtained XIVf-i, m. 100-100.5°, 94-5°, 125-6°, 130-1°; from Xd and XIIIa-d were obtained XIVj-m, m. 94-5°, 89.5-90.5°, 88.5-9.5°, and 127.5-8.5°. XIIa-c, added to dilute EtOH-HCl and allowed to stand at room temperature overnight or heated on the water bath for a short time, followed by concentration of the solution gave solids on cooling (or by the addition of H2O), which were crystallized from aqueous alc. to give XIVa-c in 80% yields. XIIc (6 g.) and saturated absolute EtOH-HCl was refluxed for 4 hrs. H2O was added to the hot solution and after cooling, the crystals were filtered off and washed with H2O to give 4.5 g. 1-[(2-nitro-3-hydroxy-4-methoxybenzoyl)amino]cyclopentane-1-carboxylic acid Et ester (XVc), m. 209-10° (decomposition) [HCONMe2 (DMF)-H2O]. XVc (3 g.) suspended in alc. was hydrogenated at arm. pressure in the presence of Pd-C to give 2.8 g. (crude) Et 1-[(2-amino-3-hydroxy-4-methoxybenzoyl)amino]cyclopentane-1-carboxylate (XVIc), m. 143-4°(alc.). Similarly, reduction of 1.26 g. XIVc gave 0.86 g. XVIc. Reduction of XIVd gave XVId, m. 141-2°. Reduction of XIVa gave XVIa, m. 180.5-1.5°. XVIa free acid (XVIIa), m. 250°, was obtained by the catalytic reduction of XIIa. To 8 g. VIIIa dissolved in hot aqueous NaOAc (2.5 g. in 120 ml. H2O) was added in small portions 31 g. Na2S2O4 until decolorization was complete. After cooling, the crystals were washed with H2O to give 5.4 g. crude 2-amino-3-hydroxy-4-methoxybenzoic acid (XVIIIa),

m. 216° (decomposition) (aqueous alc.). XVIIIa Me ester (XIXa), m. 89-90° (aqueous MeOH), was obtained by reduction of Me 2-nitro-3-hydroxy-4-methoxybenzoate. Similarly, reduction of VIIIb gave 2-amino-3-hydroxy-4-ethoxybenzoic acid (XVIIIb), m. 215.5-16.5° (decomposition) (aqueous alc.). XVIIIb Me ester (XIXb), m. 110-11° (MeOH), was obtained from the reduction of Me 2-nitro-3-hydroxy-4-ethoxybenzoate, m. 125-6° (MeOH). To a solution of 995 mg. XVIIIa in 55 ml. 0.1N NaOH was added dropwise with vigorous stirring 165 ml. of 0.1M K3Fe(CN)6. The pH was adjusted to 3-5, and stirring continued for 2 hours. The mixture was filtered, and the solids washed with H2O to give 759 mg. 2-amino-4,6dimethoxy-3-phenoxazone-1,9-dicarboxylic acid (XXa), m. >270° (decomposition) (DMF). XVIIIb gave the corresponding 4,6-diethoxy analog (XXb), m. 278° (decomposition) (DMF). XXa di-Me ester (XXI), m. 192.5-3° (DMF), and XXb di-Me ester, m. 178-9° (DMF), were obtained by oxidn, of XIXa and XIXb, resp. A mixture of 100 mg. XXI and 20 ml. 50% aqueous AcOH was refluxed 7 hrs. The product was separated by filtration and washed with alc. to give 93 mg. 2-hydroxy-4,6-dimethoxy-3-phenoxazone-1,9-dicarboxylic acid Me ester, m. 292° (decomposition) (PhNO2), depending on rate of heating. To a solution of 856 mg. XVIc in 1700 ml. warm phosphate buffer (pH 7.17) was added a solution of 1.7 g. K3Fe(CN)6 in 50 ml. H2O gradually with vigorous stirring at 40-45°. After standing for several hours, the precipitate was separated and washed once with H2O to give 712 mg. (crude) XXII (R = OMe, R1 = cyclopentylidene) (XXIIa), m. 243-4°, also prepared by air-blowing a solution of 0.3 g. XVIc in 50 ml. alc. and 50 ml. 4% (NH4)2CO3 for 20 hours. Alternatively, a solution of 0.3 g. XVIc in 25 ml. alc., and a small amount of Raney Ni or Pd-C was air-oxidized at room temperature for 20 hours, or with heated air for 4 hrs. Alc. was added as necessary to maintain the original volume The solvent was removed in vacuo, and the residue crystd from DMF to give XXIIa. The following XXII derivs. were prepared [R, R1, and m.p. (DMF) given]: MeO, CH2, 266-7°; MeO, CH2CH2, 265-6°; MeO, CHCH2Ph, 212-14°; H, CH2, 279.580.5; H, CH2CH2, 231-2°; H, CHCH2Ph, 194-5°; H, cyclopentylidene, 208-10°; Me, CH2, 267-8°; Me, CH2CH2, 256-7°; Me, CHCH2Ph, 223-4°; Me, cyclopentylidene, 265-6°; EtO, CH2, 256-8°. XVIIa (0.8 g.) in 1-1. phosphate buffer (pH 7.17) was treated with 2.1 g. K3Fe(CN)6 in 80 ml. H2O to give 0.6 g. crude N,N'-bis[2-amino-4,6-dimethoxyphenoxaz-3-one-1,9-dioyl]diglycine (XXIII), m. 257° (decomposition) (DMF). From 240 mg. XVIIa, 20 ml. 0.1N NaOH, and 20 ml. 0.1M K3Fe(CN)6 was obtained 83 mg. crude XXIII. The anal. sample from DMF m. 262° (decomposition).

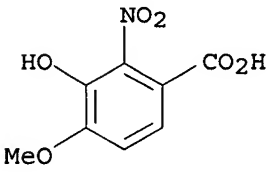
IT 3584-32-5P, Benzoic acid, 4-(benzyloxy)-3-methoxy-2-nitro- 71489-74-2P, p-Anisic acid, 3-hydroxy-2-nitro- 79025-28-8P, Veratric acid, 2-nitro- 90222-57-4P, p-Anisic acid, 2-amino-3-hydroxy- 90564-42-4P, Benzoic acid, 4-ethoxy-3-hydroxy-2-nitro- 90610-50-7P, Anthranilic acid, 4-ethoxy-3-hydroxy- 90923-43-6P, Benzoic acid, 3-ethoxy-4-methoxy-2-nitro- 90923-44-7P, Benzoic acid, 4-ethoxy-3-methoxy-2-nitro- 91134-77-9P, Benzoic acid, 3,4-diethoxy-2-nitro- 91134-78-0P, Benzoic acid, 4-isopropoxy-3-methoxy-2-nitro- 92554-37-5P, Benzoic acid, 3-(benzyloxy)-4-methoxy-2-nitro- 92868-93-4P, 3H-Phenoxazine-1,9-dicarboxylic acid, 2-amino-4,6-dimethoxy-3-oxo- 92964-19-7P, Benzoic acid, 3-(benzyloxy)-4-ethoxy-2-nitro- 93874-36-3P, 3H-Phenoxazine-1,9-dicarboxylic acid, 2-amino-4,6-diethoxy-3-oxo-
RL: PREP (Preparation)
(preparation of)

RN 3584-32-5 CAPLUS

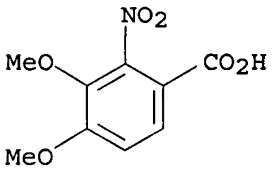
CN Benzoic acid, 3-methoxy-2-nitro-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



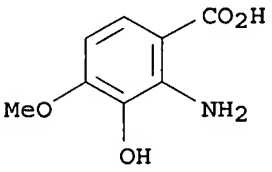
RN 71489-74-2 CAPLUS
CN Benzoic acid, 3-hydroxy-4-methoxy-2-nitro- (CA INDEX NAME)



RN 79025-28-8 CAPLUS
CN Benzoic acid, 3,4-dimethoxy-2-nitro- (9CI) (CA INDEX NAME)



RN 90222-57-4 CAPLUS
CN Benzoic acid, 2-amino-3-hydroxy-4-methoxy- (9CI) (CA INDEX NAME)



RN 90564-42-4 CAPLUS
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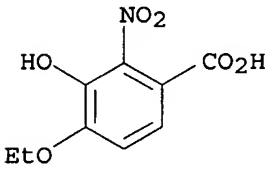
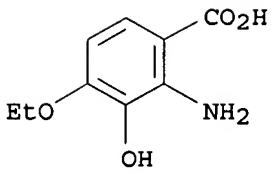
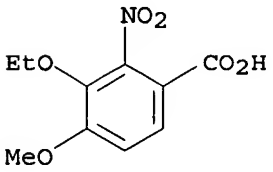


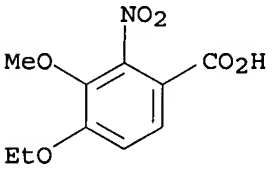
RN 90610-50-7 CAPLUS
CN Anthranilic acid, 4-ethoxy-3-hydroxy- (7CI) (CA INDEX NAME)



RN 90923-43-6 CAPLUS
CN Benzoic acid, 3-ethoxy-4-methoxy-2-nitro- (7CI) (CA INDEX NAME)



RN 90923-44-7 CAPLUS
CN Benzoic acid, 4-ethoxy-3-methoxy-2-nitro- (7CI) (CA INDEX NAME)



RN 91134-77-9 CAPLUS
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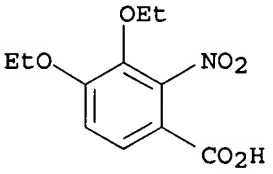
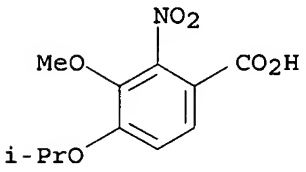
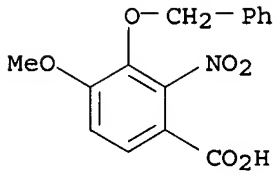


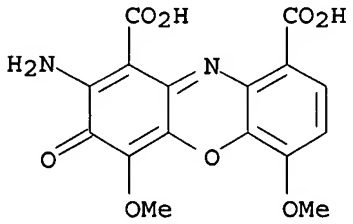
RN 91134-78-0 CAPLUS
CN Benzoic acid, 4-isopropoxy-3-methoxy-2-nitro- (7CI) (CA INDEX NAME)



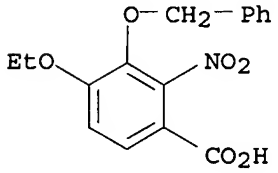
RN 92554-37-5 CAPLUS
CN Benzoic acid, 3-(benzyloxy)-4-methoxy-2-nitro- (6CI, 7CI) (CA INDEX NAME)



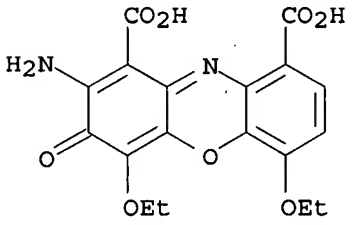
RN 92868-93-4 CAPLUS
CN 3H-Phenoxazine-1,9-dicarboxylic acid, 2-amino-4,6-dimethoxy-3-oxo- (7CI, 9CI) (CA INDEX NAME)



RN 92964-19-7 CAPLUS
CN Benzoic acid, 3-(benzyloxy)-4-ethoxy-2-nitro- (7CI) (CA INDEX NAME)



RN 93874-36-3 CAPLUS
CN 3H-Phenoxazine-1,9-dicarboxylic acid, 2-amino-4,6-diethoxy-3-oxo- (7CI) (CA INDEX NAME)



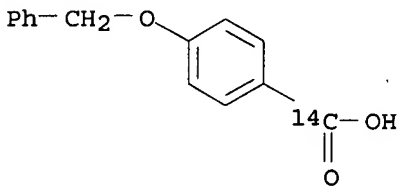
L15 ANSWER 71 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1956:4512 CAPLUS
DN 50:4512
OREF 50:863b-h
TI The synthesis of p-coumaralcoholglucoside with C-3 in the side-chain labeled with carbon-14 and of syringin
AU Kratzl, K.; Billek, G.
CS Univ. Vienna
SO Monatshefte fuer Chemie (1954), 85, 845-55
CODEN: MOCMB7; ISSN: 0026-9247
DT Journal
LA Unavailable
AB To study the biogenesis of lignin in woody plants by a previously

described method (C.A. 47, 10222e) the naturally occurring syringin (I) and the closely related p-coumaralcoholglucoside (p-ROC6H4CH:CHCH2OH where R = glucopyranosyl) (II) were synthesized with C-3 in the side chain labeled with C14. In a previously described apparatus (loc. cit.), 4-PhCH2OC6H4I (III) (1.55 g.) (prepared from 4-HOC6H4I according to Matheson and McCombie, C.A. 25, 4245) in 20 cc. dry ether was treated under N with 320 mg. BuLi in ether with stirring and in a Dry Ice-Me2CO bath, C14O2 (from 502.9 mg. BaC14O3 and 15 cc. concentrated H2SO4) passed in until no more was absorbed, the mixture treated with 20 cc. dilute HCl (1:1), the combined ether layer and ether exts. from the aqueous layer extracted with 1 g. KOH in 100 cc. H2O, the alkaline extract acidified to yield 258 mg. (44%) 4-PhCH2OC6H4C14O2H (IV), m. 188-90°. The acid chloride (V) of IV, prepared in 99% yield with SOCl2, m. 106°, was reduced in xylene solution by Pd-H (Freudenberg, et al., C.A. 46, 3514b) to impure 4-HOC6H4C14HO (VI), which was purified through conversion at pH 5-6 by m-O2NC6H4CONHNH2 to the corresponding m-nitrobenzhydrazone (43% yield), m. 282-4°, and thence oxidized in NaOH by HgCl2 to 97% VI, m. 115-16°, with the evolution of N. VI (100 mg.), 337 mg. acetobromoglucose, and 172 mg. K2CO3 in 2.5 cc. Me2CO and 1.6 cc. H2O kept 48 h. at room temperature, Me2CO distilled off in vacuo, and the residual oil dissolved in C6H6, washed with dilute KOH, dried, and distilled gave 40% sufficiently pure 4-YOC6H4C14HO (Y = tetraacetylglucosido) (VII). VII (139 mg.) diluted with 100 mg. inactive VII, warmed 1.5 h. at 100° with 138 mg. CH2(CO2H)2, 0.25 cc. C5H5N, and 0.01 cc. piperidine, the mixture treated with 25 cc. H2O, well cooled and filtered yielded 91% 4-YOC6H4C14H:CHCO2H (VIII), m. 158-61°. The acid chloride (IX) of VIII (278 mg.), prepared in 98% yield by SOCl2, m. 145-50°, in 8 cc. dry dioxane and 12 cc. dry ether reduced at -15° under N during 30 min. dropwise with 120 mg. LiAlH4 in 12 cc. ether, stirred an addnl. 30 min., and kept 2 h. at room temperature yielded, after the usual decomposition of the complex and purification, 152 mg. 4-ZOC6H4C14H:CHCH2OH (Z = partially acetylated glucosido), which was immediately hydrolyzed by Na in MeOH to 60 mg. II, m. 180-2°. By corresponding processes I, m. 190-1°, was synthesized from 4,3,5-HO(MeO)2C6H2Br (Kohn and Steiner, C.A. 41, 2704a) (3,5-di-MeO derivs. of the preceding compds., % yield, m.p. given): III (Br in place of iodine), 67, 53°; IV, 53, 155-7°; V, 80, 45°; VI, 80, 114-15°; VII, 60, 156-9°; VIII, 69, 165-6°; IX, almost 100, oil. Before the labeled I and II were ready to use in the study of lignin, the previously prepared 2-C14 labeled coniferin (C.A. 48, 4475g) (2-3 mg.) had been implanted under the bark of a spruce tree and allowed to remain several months (Freudenberg and Bittner, C.A. 48, 634e). A radioautogram and a diagram are given to show its absorption and localization in the cambium zone.

IT 10439-20-0P, Benzoic-carboxy-C14 acid, p-(benzyloxy)-
875847-40-8P, Benzoic-carboxy-C14 acid, 4-(benzyloxy)-3,5-dimethoxy-
RL: PREP (Preparation)
(preparation of)

RN 10439-20-0 CAPLUS

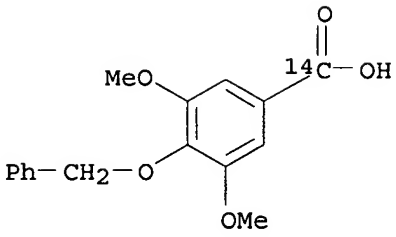
CN Benzoic-carboxy-14C acid, 4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



RN 875847-40-8 CAPLUS

CN Benzoic-carboxy-C14 acid, 4-(benzyloxy)-3,5-dimethoxy- (5CI) (CA INDEX

NAME)



L15 ANSWER 72 OF 72 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1947:814 CAPLUS
DN 41:814
OREF 41:155c-i,156a-i,157a-g
TI Amino alcohol esters of hydroxybenzoic acids
IN Christiansen, Walter G.; Harris, Sidney E.
PA E. R. Squibb & Sons
DT Patent
LA Unavailable
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2404691		19460723	US	

GI For diagram(s), see printed CA Issue.

AB Amino alc. esters of hydroxybenzoic acids, effective for inducing local anesthesia and having the general formula in which R is a bivalent aliphatic, cycloaliph., or aromatic radical providing a continuous C bridge, R' and R'' represent alkyl, aralkyl, hydroxyalkyl, or hydroxyaralkyl, or jointly represent an alkylene group, R''' represents an aliphatic, aromatic, or araliph. radical, R'''' represents H, alkyl, or an alkoxy radical, and Y is H or alkyl, are prepared by treating an aracyl halide with an amino alc. p-EtOC6H4COCl (10 g.) in 50 cc. dry benzene is treated with 6.8 g. Et2NCH2CH2OH. A precipitate forms, and the reaction is completed by heating on the H2O bath. The solution is cooled, the precipitate is filtered and treated with a slight excess of 2 N KOH, and the ester is extracted with Et2O and dried with anhydrous Na2SO4. The Et2O solution is treated with dry HCl, and the precipitate is filtered and washed with dry Et2O to yield 2-diethylaminoethyl p-ethoxybenzoate-HCl, m. 172.5-3.5°. p-EtOC6H4COCl (4.1 g.) in 15 cc. dry benzene is refluxed 30 min. with 3.5 g. AmNEtCH2CH2OH in 10 cc. dry benzene. The benzene is distilled in vacuo and the residue is dissolved in EtOH, decolorized with C, repptd. with dry Et2O, and recrystd. from Me2CO-petr. ether to give 2-(ethylamylamino)ethyl p-ethoxybenzoate-HCl, m. 108-10°. By processes essentially similar to the above described ones were prepared 2-dibutylaminoethyl p-ethoxybenzoate-HCl, m. 144.5-5.5°; 3-dibutylaminopropyl p-ethoxybenzoate-HCl, m. 85.6-6.6°; 2-diethylaminoethyl p-butoxybenzoate-HCl, m. 146°; 2-diethylaminoethyl 2-ethoxy-3-methylbenzoate-HCl, m. 97-7.5°; 2-dimethylaminoethyl p-butoxybenzoate-HCl, m. 132-3°; 2-diethylaminoethyl o-ethoxybenzoate-HCl, m. 139-9.5°; 2-diethylaminoethyl p-(2-diethylaminoethoxy)benzoate-HCl, hygroscopic crystals, m. 143°; 2-diethylaminoethyl 2-methyl-4-ethoxybenzoate-HCl, m. 101-3°; 2-diethylamino-Et 3-methyl-4-ethoxybenzoate-HCl, m. 142.5-5°; 2-diethylaminoethyl p-(2-bromallyloxy)benzoate-HCl, m. 81.5-3.5°; and 2-diethylaminoethyl 3-methoxy-4-ethoxybenzoate-HCl, m. 171.5-2.5°. A mixture of 5.5 g. Et2NCH2CH2CH2OH, 9.3 g. p-EtOC6H4COCl and 25 cc. 10% NaOH solution is vigorously stirred 0.5 h., cooled, and extracted with benzene. The benzene solution is washed with dilute NaOH and H2O, and distilled The

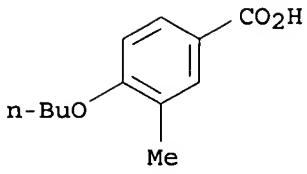
residual oil is dissolved in absolute alc. HCl and diluted with Et2O. The precipitate is filtered and recrystd. from EtOH-Et2O to give 3-diethylaminopropyl p-ethoxybenzoate-HCl, m. 148.5-9.5°. 2-Diethylaminocyclohexanol (6.8 g.) in 75 cc. dry benzene is treated with 10 g. finely powdered anhydrous K2CO3 and then with 7.3 g. p-EtOC6H4COCl. The mixture is refluxed several hrs. and treated with 100 cc. H2O and 100 cc. benzene. The benzene layer is removed and purified and treated as in the above preparation to yield 2-diethylaminocyclohexyl p-ethoxybenzoate-HCl, m. 184-5°. In substantially the same manner were prepared 2-hydroxy-3-diethylaminopropyl p-ethoxybenzoate-HCl, m. 120-6°; and (N-phenacyl-N-ethylamino)ethyl p-ethoxybenzoate-HCl, white crystals. (HOCH2CH2)2NEt (6.7 g.) in 100 cc. dry benzene is treated with 14 g. anhydrous K2CO3 and then with 9.2 g. p-EtOC6H4COCl, and the mixture is refluxed with stirring for 2 h. The mixture is filtered, the benzene evaporated, and the residue distilled in vacuo to yield 2-[ethyl(2-hydroxyethyl)amino]ethyl p-ethoxybenzoate, thick, colorless oil, b8 218-25°; HCl salt, hygroscopic crystals. In similar manner were prepared 2-diethylaminoisohexyl p-ethoxybenzoate, b2.5 175-85°, b5 193-5°; 3-diethylamino-2-hydroxypropyl p-butoxybenzoate-HCl, mixture of 2 isomers, m. 79-96°; 2-[ethyl(2-hydroxyethyl)amino]ethyl p-butoxybenzoate, b3 216-20°; HCl salt, hygroscopic. A mixture of 1.5 g. Me2NCH2CEt(OH)CH2NMe2 in 5 cc. CHCl3 and 1.6 g. p-EtOC6H4CO2H in 5 cc. CHCl3 is heated 5 min. on the steam bath. Dry _ Et2O is added, and the precipitate is filtered, washed, and dried to give 1,1-bis(dimethylaminomethyl) Pr p-ethoxybenzoate-HCl, white crystalline powder, m. 121-1.5°. In like manner was prepared 1,1-bis(dimethylaminomethyl)propyl p-butoxybenzoate-HCl, m. 111°. m-EtOC6H4COCl (11.5 g.) in 50 cc. dry benzene is mixed with 14.5 Et2NCH2CH2OH in 50 cc. dry benzene, and the mixture heated on the steam bath 1 h. The precipitate is filtered, and the benzene filtrate is distilled The residue is distilled in vacuo to give 2-diethylaminoethyl m-ethoxybenzoate, b2 163-75°. This was dissolved in alc. HCl, and repptd. with Et2O to yield the HCl salt, m. 125-5.5°. Similarly were prepared 2-diethylaminoethyl p-(2-ethoxyethoxy)benzoate-HCl, m. 102-3.5°; 2-diethylaminoethyl p-propoxybenzoate, b4 160-5° (HCl salt, m. 135-6°); 2-diethylaminoethyl p-isopropoxybenzoate-HCl, m. 125.5°; and 2-diethylaminoethyl p-allyloxybenzoate, b4 165-75° (HCl salt, m. 130°). A mixture of 2.5 g. p-EtOC6H4CO2CH2CH2CH:CHBr, 5.5 g. Et2NH, and 15 cc. benzene is heated in a sealed tube at 125-35° for 8 h. After cooling, the mixture is treated with H2O and extracted with Et2O. The Et2O extract is washed with H2O, dried, and distilled on the steam bath, finally under reduced pressure. The residue is dissolved in alc. HCl and precipitated with Et2O. Washing with dry Et2O of the oily precipitate yields 4-diethylamino-4-butenyl p-ethoxybenzoate-HCl, yellowish white crystals, m. 146-7°. Heating Et2NCH2CMe2CH2OH with p-EtOC6H4COCl in dry Me2CO yields 2,2-dimethyl-3-diethylaminopropyl p-ethoxybenzoate-HCl, m. 122-4°. 3,4-Me(BuO)C6H3COCl (1.05 g.) and 1.25 g. (Me2NCH2)2C(OH)CH2CH2Ph in 10 cc. CHCl3 are refluxed for a few min., treated with dry Et2O to incipient precipitation, and allowed to stand. The crystalline precipitate which seps. after some time is filtered and washed with dry Et2O to give 1,1-bis(dimethylaminomethyl)-3-phenylpropyl 3-methyl-4-butoxybenzoate-HCl, m. 161-2°. Similarly were prepared 2,2'-bis(dimethylamino)isopropyl p-propoxybenzoate mono- and di-HCl salts, m. 208°; 3-dimethylaminopropyl 3-methyl-4-butoxybenzoate-HCl, white crystalline powder, m. 125.5-6.5°; 3-dimethylaminopropyl p-(2-phenylethoxy)benzoate-HCl, m. 156.5-7-5°; and 1-methyl-1-(dimethylaminomethyl)amyl 3-methyl-4-butoxybenzoate-HCl, m. 126-31°. p-EtOC6H4CO2CH2CH2NEtCH2COPh (0.9 g.) in 60 cc. EtOH containing 0.3 g. PtO is shaken 8 h. under a pressure of 35 lb. H, filtered, and the filtrate is concentrated to a small volume and diluted with Et2O. The crystalline precipitate is filtered, washed with Et2O, and dried in vacuo over CaCl2

to give 2-[ethyl(2-phenyl-2-hydroxyethyl)amino]ethyl p-ethoxybenzoate-HCl. 2-Diethylaminoethyl p-(p-aminobenzyloxy) benzoate-HCl, m. 185-7°, is prepared in the same manner, p-HOC6H4CO2CH2CH2NEt2 (0.4 g.) in 50 cc. dry Me2CO containing 15 g. anhydrous K2CO3 is treated with 5.5 g. p-O2NC6H4CH2Br, and the mixture is refluxed 12 h. The mixture is filtered, and the Me2CO distilled from the filtrate. The residue is treated with alc. HCl and diluted with Me2CO and Et2O. The precipitate is recrystd. from Me2CO-Et2O to give 2-diethylaminoethyl p-(p-nitrobenzyloxy)benzoate-HCl, m. 145-6°. In addition, 21 other similar compds. are cited, but no phys. properties are recorded. The prepns. of many intermediates used in preparing the above compds. are described. A solution of 3.5 g. Na in 100 cc. absolute EtOH is treated first with 25 g. 2,3-HO(MeO)C6H3CO2Et and then with 20 g. EtBr, and the solution is boiled until neutral to moist litmus. The mixture is filtered, and the EtOH is removed from the filtrate. The residue is fractionated to yield Et 2-ethoxy-3-methylbenzoate, b6 116-18°, which upon hydrolysis with alc. NaOH yielded 2-ethoxy-3-methylbenzoic acid, oily precipitate, which was extracted with ether. The ether was removed and the residue treated with SOCl2 to give 2-ethoxy-3-methylbenzoyl chloride, b2.5 102-5°. p-(2-Phenylethoxy)benzoic acid, white powder, m. 163-4° (chloride, b5 215-30°), and 3-methyl-4-(2-phenylethoxy) benzoic acid, m. 150-2° (chloride, b1 210-15°), were prepared in essentially the same manner. p-HOC6H4CO2Me (13 g.) in 35 cc. Me2CO is treated with 15 g. anhydrous K2CO3, the mixture is refluxed and stirred, treated with 13 g. Et2NCH2CH2Cl, heated, stirred 15 h., filtered, and the filtrate concentrated by distillation The residue is treated with excess NaOH and boiled until saponification is complete. The solution is extracted with Et2O, and the aqueous solution is evaporated to dryness in vacuo. The residue is extracted with absolute EtOH, the extract filtered, the filtrate evaporated to dryness, and the residue recrystd. from MeOHEt2O to give p-(2-diethylaminoethoxy)benzoic acid-HCl, white needles, m. 160-1°. Treatment with PCl5 yields p-(2-diethylaminoethoxy)benzoyl chloride-HCl, m. 143°. In similar manner were prepared 2-methyl-4-ethoxybenzoyl chloride, colorless liquid, b3 138-40°; 3-methyl-4-ethoxybenzoyl chloride, colorless liquid, b6 147-52°; p-(2-ethoxyethoxy)benzoic acid, m. 131-2° (chloride, b5 150-60°); p-(2-bromoallyloxy)benzoic acid, m. 200° (decomposition) (chloride, b5 160-70°); 3-methoxy-4-ethoxybenzoyl chloride, b5 147-50°, m. 72°, and 3-methyl-4-butoxybenzoic acid, white plates from 60% EtOH, m. 144-6° (chloride, b1.5 144-54°). A mixture of 5.5 g. dry p-EtOC6H4CO2Na, 8 g. BrCH:CHCHBrMe, and 10 g. dry xylene is heated in a sealed tube at 165-70° for 6 h. The contents of the tube are extracted with dilute EtOH and Et2O. The Et2O is washed with H2O, dried over Na2SO4, and distilled The oily residue is fractionated in a high vacuum to yield 3-bromo-1-butenyl p-ethoxybenzoate, b3 165-75°. A mixture of 9.95 g. PhCOCH2Cl, 4.4 g. EtNHCH2CH2OH, and 100 cc. benzene is refluxed 3 h. On adding 10 g. K2CO3, a vigorous evolution of CO2 ensues. The suspension is further refluxed 4 h. and filtered. The filtrate is treated with HCl in Et2O. The reddish brown semisolid which seps. is filtered, washed with Et2O, and dried in a vacuum over CaCl2 to yield the very hygroscopic N-phenacyl-N-ethyl-2-aminoethanol-HCl, which is treated with p-EtOC6H4COCl in benzene in the presence of K2CO3 in the regular manner to give N-phenacyl-N-ethyl-2-aminoethyl p-ethoxybenzoate-HCl, white crystals.

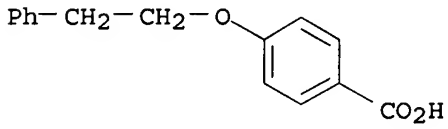
IT 872827-91-3, m-Toluic acid, 4-butoxy-
(and derivs.)

RN 872827-91-3 CAPLUS

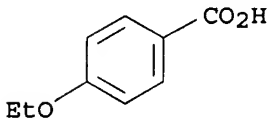
CN m-Toluic acid, 4-butoxy- (5CI) (CA INDEX NAME)



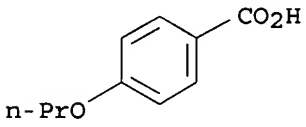
IT 30762-06-2, Benzoic acid, p-phenethyloxy-
(and esters)
RN 30762-06-2 CAPLUS
CN Benzoic acid, 4-(2-phenylethoxy)- (9CI) (CA INDEX NAME)



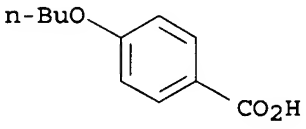
IT 619-86-3, Benzoic acid, p-ethoxy- 5438-19-7, Benzoic acid, p-propoxy-
(esters)
RN 619-86-3 CAPLUS
CN Benzoic acid, 4-ethoxy- (CA INDEX NAME)



RN 5438-19-7 CAPLUS
CN Benzoic acid, 4-propoxy- (CA INDEX NAME)



IT 1498-96-0, Benzoic acid, p-butoxy-
(esters with amino alc. derivs., and their salts)
RN 1498-96-0 CAPLUS
CN Benzoic acid, 4-butoxy- (CA INDEX NAME)



IT 92315-60-1, m-Toluic acid, 4-ethoxy-, 2-diethylaminoethyl esters
(hydrochlorides)
RN 92315-60-1 CAPLUS
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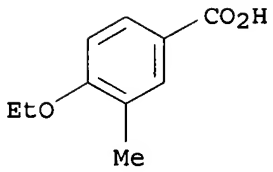
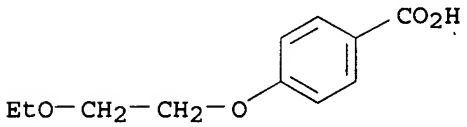


IT 40782-64-7P, Benzoic acid, p-(2-ethoxyethoxy)- 59931-28-1P , Benzoic acid, p-(2-diethylaminoethoxy)-, hydrochloride 872827-91-3P, m-Toluic acid, 4-butoxy- 874514-53-1P, m-Toluic acid, 4-phenethyloxy- 875846-82-5P, Benzoic acid, p-(2-bromoallyloxy)-
RL: PREP (Preparation)
(preparation of)

RN 40782-64-7 CAPLUS
CN Benzoic acid, 4-(2-ethoxyethoxy)- (9CI) (CA INDEX NAME)



RN 59931-28-1 CAPLUS
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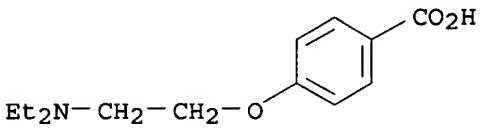
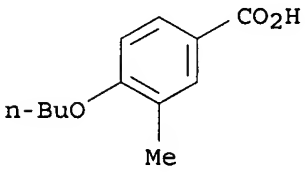
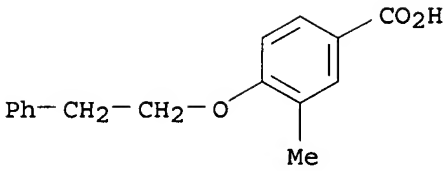


RN 872827-91-3 CAPLUS
CN m-Toluic acid, 4-butoxy- (5CI) (CA INDEX NAME)



RN 874514-53-1 CAPLUS
CN m-Toluic acid, 4-phenethyloxy- (5CI) (CA INDEX NAME)



RN 875846-82-5 CAPLUS
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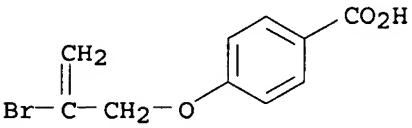

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Executing the logoff script...

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	387.82	732.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-56.16	-56.16

STN INTERNATIONAL LOGOFF AT 17:39:04 ON 14 SEP 2007